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REMARKS

Reconsideration of this patent application is respectfully requested in view of the foregoing amendments, and the following remarks.

The amendments to this patent application are as follows. Amendments have been made to the drawings, the Specification, the Abstract, and the claims so as to overcome all of the various formal rejections by the Patent Examiner.

The amendments to the drawings are to cancel the drawings now on file and to replace them with a revised set of drawings for FIG. 1 to 11. These revised drawings have deleted any reference to a total of only 10 drawing sheets and have been amended to refer to a total of 11 drawing sheets. Also these revised drawings have used "Prior Art" to identify each one of FIGS. 3a, 3b, 10a and 10b.

The Substitute Specification has been amended as follows. On Page 1, the Substitute Specification has been amended to delete any reference to the PCT patent application, as required by the Patent Examiner. The Substitute Specification on Page 30

has been amended in order to correct the spelling of the word "photometric". The Substitute Specification on Page 32 has been amended to refer to "figure 1" in line 6. The Substitute Specification on Page 39 has been amended to revise the equations to show larger print for the subscripts.

The Abstract of the Disclosure has been amended to delete "legal phraseology" and "purported merits", objected to by the Patent Examiner. Thus the word "said" has been changed to "the". Also the language "which are useful" and "that can be used", have been cancelled.

The amendments to the claims are as follows.

The Patent Examiner had objected to claim 92 in line 3, because the terminology "the infrared active components" lacks clear antecedent basis. Thus claim 92 has now been amended to provide proper antecedent basis.

Claim 96 has been amended to correct a minor typographical error concerning the density.

The Patent Examiner had objected to claim 98, in lines 17-18, because the terminology "the radiation receiver" has a different antecedent basis which is "at least one radiation receiver". Thus claim 98 has now been amended to provide the proper antecedent basis.

The Patent Examiner objected to claim 105, in lines 5 and 7, because reference numerals were not deleted. Thus claim 105 has been amended in order to delete these reference numerals.

The Patent Examiner objected to claim 108, in lines 2-4 of this claim which now recites "...wherein the probe cell is sweepable with an infrared inactive gas, preferably for carrying out a null measurement..." which is still allegedly indefinite because it is not clear as to the range of the probe cell being swept with an infrared inactive gas. Thus claim 108 has been amended to delete the "preferably" terminology.

The Patent Examiner has repeated his objection with respect to the terminology of industry standards being employed in claims 87, 88, 89 and 94.

With regard to the formal rejection by the Patent Examiner regarding these claims, relating to the use of standard calculation methods, the following should be noted:

The standard calculation methods used in the present patent application are both shown in ISO 12213, specifically AGA8-92DC in ISO 12213-2 and GERG in ISO 12213-3. No English version of the DVGW working paper is known, but it is derived from 12213. This means that the English language document ISO 12213 is the relevant document. Enclosed is a copy of ISO 12213 in English.

At present, only the two methods mentioned are of practical significance, since they produce the best results. An older method is the method according to AGA NX19, which is allowed to be used only at low pressures, for example. However, a new GERG2 method is currently being developed, which is superior to the existing equations and is also supposed to be elevated to a standard. Moreover, the time when this will happen is not known as yet. However, this method will differ from the previous method also in terms of the designation. Hence the uncertainty that exists from the point of view of the Patent Examiner, with regard to the scope of the standard referred to, in each instance, should actually no longer exist. It is pointed out to

the Patent Examiner, with regard to the enclosure, that it is true that new standards can be developed. These new standards are also being used in place of the old standards, so that even in the relevant art, no lack of clarity can occur with regard to the standard that is actually meant. For these reasons, the formal ground rejection with regard to the precise content of the claims is respectfully submitted to have been overcome.

A restriction of the claims only to the methods mentioned is not necessary, since there is no prior art rejection. Also one skilled in the art would clearly understand the meaning of all the art recognized terminology.

However, the standard calculation method, as an iteration method according to the present invention, is also completely independent of the real gas calculation method actually being used. Instead, any algorithm for describing the real gas behavior of natural gas that yields one of the following variable is suitable:

real gas factor Z = compression factor Z

compressibility K = compressibility ratio K

Based upon all of the above-discussed amendments to the Abstract, the Specification, the drawings, and all the claims, the present patent application is now in complete compliance with all the requirements of 35 U.S.C. 112. Withdrawal of this ground of rejection is respectfully requested.

A prompt notification of allowability is respectfully requested.

Respectfully submitted,

DIETER STIRNBERG ET AL-1 PCT

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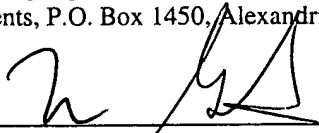
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- Enclosures: 1) Drawing Replacement Sheets for FIG. 1 to 11.
2) Copy of ISO 12213 in English

I hereby certify that this correspondence is being deposited with the U.S. Postal Service as first class mail in an envelope addressed to: Commissioner of Patents, P.O. Box 1450, Alexandria, VA 22313-1450, on June 23, 2004



Maria Guastella

INTERNATIONAL STANDARD

ISO
12213-1

First edition
1997-12-01

Natural gas — Calculation of compression factor —

Part 1: Introduction and guidelines

Gaz naturel — Calcul du facteur de compression —

Partie 1: Introduction et directives

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Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

Draft International Standards adopted by the technical committees are circulated to the member bodies for voting. Publication as an International Standard requires approval by at least 75 % of the member bodies casting a vote.

International Standard ISO 12213-1 was prepared by Technical Committee ISO/TC 193, *Natural gas*, Subcommittee SC 1, *Analysis of natural gas*.

ISO 12213 consists of the following parts, under the general title *Natural gas* — *Calculation of compression factor*.

- *Part 1: Introduction and guidelines*
- *Part 2: Calculation using molar-composition analysis*
- *Part 3: Calculation using physical properties*

Annex A forms an integral part of this part of ISO 12213. Annexes B and C are for information only.

Natural gas — Calculation of compression factor —

Part 1:

Introduction and guidelines

1 Scope

This International Standard specifies methods for the calculation of compression factors of natural gases, natural gases containing a synthetic admixture and similar mixtures at conditions under which the mixture can exist only as a gas.

The standard is in three parts: part 1 gives an introduction and provides guidelines for the methods of calculation described in parts 2 and 3.

Part 2 gives a method for use where the detailed molar composition of the gas is known. Part 3 gives a method for use where a less detailed analysis, comprising superior calorific value (volumetric basis), relative density, carbon dioxide content and (if non-zero) hydrogen content, is available.

Both methods are applicable to dry gases of pipeline quality within the range of conditions under which transmission and distribution, including metering for custody transfer or other accounting purposes, are normally carried out. In general, such operations take place at temperatures between about 263 K and 338 K (approximately -10°C to 65°C) and pressures not exceeding 12 MPa (120 bar). Within this range, the uncertainty of prediction of both methods is about $\pm 0,1\%$ provided that the input data, including the relevant pressure and temperature, have no uncertainty.

NOTE — Pipeline quality gas is used in this International Standard as a concise term for gas which has been processed so as to be suitable for use as industrial, commercial or domestic fuel. Although there is no formal international agreement upon the composition and properties of a gas which complies with this concept, some quantitative guidance is provided in 5.1.1. A detailed gas quality specification is usually a matter for contractual arrangements between buyer and seller.

The method given in part 2 is also applicable (with increased uncertainty) to broader categories of natural gas, including wet or sour gases, within a wider range of temperatures and to higher pressures, for example at reservoir or underground storage conditions or for vehicular (NGV) applications.

The method given in part 3 is applicable to gases with a higher content of nitrogen, carbon dioxide or ethane than normally found in pipeline quality gas. The method may also be applied over wider ranges of temperature and pressure but with increased uncertainty.

For the calculation methods described to be valid, the gas must be above its water and hydrocarbon dewpoints at the prescribed conditions.

The standard gives all of the equations and numerical values needed to implement both methods. Verified computer programmes are available (see annex B).

2 Normative references

The following standards contain provisions which, through reference in this text, constitute provisions of this part of ISO 12213. At the time of publication, the editions indicated were valid. All standards are subject to revision, and parties to agreements based on this part of ISO 12213 are encouraged to investigate the possibility of applying the most recent editions of the standards indicated below. Members of IEC and ISO maintain registers of currently valid International Standards.

ISO 6976:1995, *Natural gas — Calculation of calorific values, density, relative density and Wobbe index from composition*.

ISO 13443:1996, *Natural gas — Standard reference conditions*.

3 Definitions

For the purposes of the various parts of this International Standard, the following definitions apply.

3.1 compression factor, Z : The ratio of the volume of an arbitrary mass of gas, at a specified pressure and temperature, to the volume of the same mass of gas under the same conditions as calculated from the ideal-gas law, as follows:

$$Z = V_{\text{m}}(\text{real}) / V_{\text{m}}(\text{ideal}) \quad \dots (1)$$

$$\text{where } V_{\text{m}}(\text{ideal}) = RT/p \quad \dots (2)$$

$$\text{Thus, } Z(p, T, y) = pV_{\text{m}}(p, T, y)/(RT) \quad \dots (3)$$

where

p is the absolute pressure;

T is the thermodynamic temperature;

y is a set of parameters which uniquely characterizes the gas (in principle, the latter may be the complete molar composition or a distinctive set of dependent physico-chemical properties, or a mixture of both);

V_{m} is the molar volume of the gas;

R is the molar gas constant in coherent units.

The compression factor is a dimensionless quantity usually close to unity.

NOTE — The terms "compressibility factor" and "Z-factor" are synonymous with compression factor.

3.2 density, ρ : The mass of a given quantity of gas divided by its volume at specified conditions of pressure and temperature.

3.3 molar composition: The term used when the proportion of each component in a homogeneous mixture is expressed as a mole (or molar) fraction, or mole (molar) percentage, of the whole.

Thus the mole fraction x_i of component i is the ratio of the number of moles of component i in a given volume of a mixture to the total number of moles of all the components in the same volume of the mixture. One mole of any chemical species is the amount of substance which contains the relative molecular mass in grams. A table of recommended values of relative molecular masses is given in ISO 6976.

For an ideal gas, the mole fraction (or percentage) is identical to the volume fraction (or percentage), but this is not in general a sufficiently accurate approximation to real-gas behaviour for the purposes of this International Standard.

3.4 molar calorific value, H : The amount of heat which would be released by the complete combustion in air of the hydrocarbons in one mole of natural gas in such a way that the pressure at which the reaction takes place remains constant and all the products of combustion are returned to the same specified temperature as that of the reactants, all of these products being in the gaseous state except for water formed by combustion, which is condensed to the liquid state at the specified temperature.

Note that the molar calorific value only includes the hydrocarbons in the natural gas, i.e. inert components (primarily nitrogen, carbon dioxide and helium) and other combustible components (such as hydrogen and carbon monoxide) are excluded.

The specified temperature is 298,15 K (25 °C) and the reference pressure is 101,325 kPa.

The term "molar heating value" is synonymous with "molar calorific value".

3.5 superior calorific value, H_S (volumetric basis): The amount of heat which would be released by the complete combustion in air of all the combustible components in unit volume of natural gas in such a way that the pressure at which the reaction takes place remains constant and all the products of combustion are returned to the same specified temperature as that of the reactants, all of these products being in the gaseous state except for water formed by combustion, which is condensed to the liquid state at the specified temperature.

Note that the superior calorific value includes all the combustible components in the natural gas.

The reference temperature at which the volume is measured is 273,15 K (0 °C) and the specified temperature at which combustion takes place is 298,15 K (25 °C). The reference pressure is 101,325 kPa.

NOTE — Annex D of part 3 of this International Standard gives conversion factors which enable superior calorific values and relative densities determined at other reference or specified temperatures, and other reference pressures, including the ISO standard reference conditions (see ISO 13443), to be used as input data for the calculation method described.

The terms "gross", "higher", "upper" and "total calorific value" and "heating value" are synonymous with "superior calorific value".

3.6 relative density, d : The ratio of the mass of a given volume of natural gas to the mass of dry air of standard composition which would be contained in the same volume at the same reference conditions of pressure and temperature.

The relative density includes all the components of the natural gas.

NOTE — The standard composition of dry air is given in ISO 6976.

In this International Standard, the reference temperature is 273,15 K (0 °C) and the reference pressure is 101,325 kPa (see note in 3.5).

The term "specific gravity" is synonymous with "relative density".

3.7 uncertainty of a predicted compression factor, $\pm \Delta Z$: The range of values $Z - \Delta Z$ to $Z + \Delta Z$ within which the (unknown) true value is expected to lie with a confidence level of 95 %. This uncertainty may be expressed either as an absolute value or as a percentage.

Estimates of the 95 % confidence limits are, to the extent that this is practicable, established by comparison of test data of low uncertainty with calculated values of Z .

4 General principles

The methods recommended use equations which are based on the concept that any natural gas may be uniquely characterized for calculation of its volumetric properties either by component analysis or by an appropriate and distinctive set of measurable physical properties. These characteristics, together with the pressure and temperature, are used as input data for the methods.

In the sense that the volumetric behaviour of a gas mixture derives directly from the numbers and types of molecular interactions (collisions) which take place, a method which explicitly recognizes each molecular constituent of the mixture, and its proportion of the whole, is to some degree more fundamental than alternatives.

The method given in part 2 of this International Standard uses a detailed molar-composition analysis in which all constituents present in amounts exceeding a mole fraction of 0,000 05 should be represented. The sum of the mole fractions used should be unity to within 0,000 1. For a typical distributed (pipeline quality) gas, this includes all alkane hydrocarbons up to about C₇ or C₈ together with nitrogen, carbon dioxide and helium. For gases containing a synthetic admixture, hydrogen, carbon monoxide and ethylene are also likely to be significant components. For broader categories of gas, other components such as water vapour and hydrogen sulfide need to be taken into consideration.

The equation recommended is known as the AGA8 detailed characterization equation, and will be referred to hereafter as the AGA8-92DC equation [1] (see annex C). It is a revision of the equation described in AGA Report No. 8 [2].

The method given in part 3 of this International Standard uses two distinct physical properties, namely superior calorific value and relative density, together with the carbon dioxide content.

NOTE — In principle, any three from superior calorific value, relative density, carbon dioxide content and nitrogen content may be used, the calculation methods being essentially equivalent. However, the set comprising the first three is preferred for this International Standard. The reader interested in the use of alternative input variables is referred to the GERG TMS documentation [3].

This method is particularly useful in the common situation where a complete molar composition is not available, but may also be preferred for its relative simplicity. For gases containing a synthetic admixture, the amount of hydrogen needs to be known.

The equation recommended is known as the SGERG-88 equation [3]. This equation is derived from the MGERG-88 equation [4], which uses a detailed molar analysis to characterize the gas.

The evaluation of both the AGA8-92DC and the SGERG-88 equations has been carried out using a large databank of high-accuracy ($\pm 0,1\%$) compression factor measurements (most of which are traceable to the relevant international metrological standards), compiled for the purpose by the Groupe Européen de Recherches Gazières [5] and the Gas Research Institute [6] [7]. Within the transmission and distribution pressure and temperature ranges, the equations are of essentially identical performance.

5 Guidelines

5.1 Pipeline quality natural gases

5.1.1 Pipeline quality gas

To make a definitive quantitative specification of what does or does not represent pipeline quality natural gas is, for several reasons, an elusive and contentious objective. Nevertheless, most transmission and distribution engineers are familiar with the general concept and will normally know whether any particular natural gas falls within the scope of this term. The following is therefore intended simply to provide summary guidance for any other users, rather than to formalize criteria for pipeline quality gas.

Pipeline quality gas is taken to consist predominantly (mole fraction greater than 0,70) of methane and to have a superior calorific value normally within the range 30 MJ·m⁻³ to 45 MJ·m⁻³ (see table 1). Nitrogen and carbon dioxide are the main diluents (each up to a mole fraction of about 0,20).

Ethane (up to a mole fraction of about 0,10), propane, butanes, pentanes and higher alkanes will usually be present in steadily decreasing amounts. Minor amounts of helium, benzene and toluene may be present at mole fractions of less than 0,001. For natural gases with a synthetic admixture, hydrogen and carbon monoxide may be present in mole fractions of up to about 0,10 and 0,03, respectively, and there may be small amounts of ethylene. No other component, such as those found in wet and sour gases (for example water vapour, hydrogen sulfide or oxygen), is

normally present in greater than trace amounts, and there should be no aerosol, liquid or particulate matter present. Minor and trace components should be treated as specified in part 2 of this International Standard.

This way of defining pipeline quality gas is not intended to exclude natural gases of other compositions from being transported through pipelines.

The limits allowable for the purpose of this International Standard are given in table 1.

Table 1 — Allowable limits for mole fractions of components

| Component | Mole fraction |
|-----------------------------------|------------------|
| Main components | |
| Methane | $\geq 0,70$ |
| Nitrogen | $\leq 0,20$ |
| Carbon dioxide | $\leq 0,20$ |
| Ethane | $\leq 0,10$ |
| Propane | $\leq 0,035$ |
| Butanes | $\leq 0,015$ |
| Pentanes | $\leq 0,005$ |
| Hexanes | $\leq 0,001$ |
| Heptanes | $\leq 0,000\ 5$ |
| Octanes and above | $\leq 0,000\ 5$ |
| Hydrogen | $\leq 0,10$ |
| Carbon monoxide | $\leq 0,03$ |
| Helium | $\leq 0,005$ |
| Water | $\leq 0,000\ 15$ |
| Minor and trace components | |
| Ethylene | $\leq 0,001$ |
| Benzene | $\leq 0,000\ 5$ |
| Toluene | $\leq 0,000\ 2$ |
| Argon | $\leq 0,000\ 2$ |
| Hydrogen sulfide | $\leq 0,000\ 2$ |
| Oxygen | $\leq 0,000\ 2$ |
| Total unspecified components | $\leq 0,000\ 1$ |

5.1.2 Transmission and distribution metering

The main use of this International Standard is expected to be for the calculation of compression factors in applications concerned with transmission and distribution of pipeline quality gases. The range of conditions encountered in such applications varies from country to country, but almost all will be covered by the limits

$$263\text{ K} \leq T \leq 338\text{ K}$$

$$0\text{ MPa} < p \leq 12\text{ MPa}$$

The methods given in parts 2 and 3 apply with equal validity for all conditions within these limits.

5.1.3 Calculation using a molar-composition analysis

The AGA8-92DC equation may be used for any pipeline quality gas for which a detailed molar-composition analysis is available. The components which the analysis should include are: methane, nitrogen, carbon dioxide, carbon monoxide, hydrogen, helium, ethane, propane, butanes, pentanes, hexanes, and (if present at mole fractions greater than 0,000 05) higher hydrocarbons up to C₁₀. The amount of each minor or trace component specified in the lower part of table 1 should be demonstrably within the relevant limit. Any non-negligible amount of a minor or trace component should be treated in the manner specified in part 2 of this International Standard.

Within the ranges quoted in 5.1.2, the calculated compression factor values have the same status (i.e. equal validity) as those calculated from superior calorific value, relative density and carbon dioxide content.

The method may be used in all applications where the composition is subject to regular or semi-continuous determination.

5.1.4 Calculation using physical properties

The SGERG-88 equation may be used for any pipeline quality natural gas having a superior calorific value in the range 30 MJ·m⁻³ to 45 MJ·m⁻³, a relative density in the range 0,55 to 0,80, a known carbon dioxide content and a known hydrogen content.

Within the range quoted in 5.1.2, the calculated compression factor values have the same status (i.e. equal validity) as those calculated from a complete molar-composition analysis.

The method may be used in all applications where H_s and d are subject to regular or continuous determination.

5.1.5 Manufactured gases

Neither the AGA8-92DC method given in part 2 nor the SGERG-88 method given in part 3 is specifically intended for use with manufactured (synthetic) gases, as these may contain substantial amounts of chemical species which are atypical of natural gases, or common species in atypical proportions (see 5.2.3).

Either method may, however, be used if it can be demonstrated that the composition of the synthetic gas closely matches that of a possible true natural gas, all of the components falling within the ranges of concentration given in 5.1.1, with hydrocarbons above butane (C₄) either absent or decreasing regularly with increasing carbon number. In the sense that hydrocarbons above C₄ are virtually absent, liquefied natural gas may fall within this category.

In addition, the SGERG-88 method may be used with natural gases containing a coke-oven gas mixture up to the specified concentration limit for hydrogen. The method may not, however, be used with "undiluted" coke-oven gas.

5.1.6 Predictive uncertainty

Given exact values of all of the relevant input variables, the methods given in parts 2 and 3 are both expected to achieve an uncertainty of prediction of $\pm 0,1$ % in the compression factor for the entire ranges of composition and physical properties given in 5.1.1 for pipeline quality gas, and of pressure and temperature quoted in 5.1.2 for transmission and distribution applications.

The only exceptions to this are as follows. For the prediction of Z , by the method given in part 3, for gases containing more than a 0,15 mole fraction of nitrogen or 0,05 of carbon dioxide (up to the relevant limits of 0,20), an uncertainty within $\pm 0,10$ % is only maintained up to about 10 MPa for nitrogen and 6 MPa for carbon dioxide (see 5.2.2).

It is stressed, however, that any uncertainty in the input variables adds further uncertainty to the result. The sensitivity of the result to the accuracy of the input variables depends significantly, and in a complicated manner, upon:

- a) the magnitude of each input variable;
- b) the degree of independence of each input variable from the values of other input variables.

In most cases, the greatest sensitivity of the result towards all of the input variables is found at the upper extremity of the pressure range (12 MPa) and the lower extremity of the temperature range (263 K).

As a general guideline only, uncorrelated uncertainties of the variables listed in table 2 may contribute to an additional uncertainty of the result of about $\pm 0,1$ % at 6 MPa and within the temperature range 263 K to 338 K.

Table 2 — Allowable uncertainties of input variables for $\Delta Z < 0,1 \%$

| Input variable | Allowable uncertainty |
|-----------------------------------|---|
| Calorific value | $\pm 0,06 \text{ MJ}\cdot\text{m}^{-3}$ |
| Relative density | $\pm 0,001 \text{ 3}$ |
| Temperature | $\pm 0,15 \text{ K}$ |
| Pressure | $\pm 0,02 \text{ MPa}$ |
| Mole fraction of | |
| Inerts | $\pm 0,001$ |
| methane | $\pm 0,001$ |
| ethane | $\pm 0,001$ |
| propane | $\pm 0,000 \text{ 5}$ |
| butane | $\pm 0,000 \text{ 3}$ |
| pentanes plus higher hydrocarbons | $\pm 0,000 \text{ 1}$ |
| hydrogen and carbon monoxide | $\pm 0,001$ |

Thus, the choice of calculation method should take into account not only the availability of an appropriate form of input data, but also its accuracy. In circumstances where it is unclear whether the instrumental accuracy is sufficient, the user should carry out sample calculations of the compression factor at the highest pressure and lowest temperature of interest in order to establish, for gases typical of the application in question, the sensitivity to independent small variations of all input variables.

5.1.7 Wider ranges of pressure and temperature

Both the AGA8-92DC and SERG-88 equations degrade in accuracy outside the primary ranges of pressure and temperature given in 5.1.2.

However, the AGA8-92DC equation is generally expected to extrapolate beyond these ranges more accurately than the SERG-88 equation, and consequently would often be the preferred alternative for applications outside the normal range of transmission and distribution conditions.

The predictive uncertainty of the AGA8-92DC equation depends strongly upon both the composition of the gas and the conditions under consideration. Further advice is given in part 2 concerning the uncertainty of prediction to be expected at any selected conditions. This uncertainty may sometimes be almost as low as that for the transmission and distribution region, but at extremes of temperature or pressure will be significantly greater. Because of the lack of high-accuracy test data, it is extremely difficult to assess the uncertainty.

5.2 Other gases and other applications

5.2.1 Introduction

Not all fluids with which the gas engineer may typically have to deal, and for which he may need to know compression factors, are natural gases of pipeline quality. For example, unprocessed (well-head) or partially processed natural gases do not normally fall within the scope of the term pipeline quality gas as defined in 5.1.1, for which this International Standard is primarily intended. Nor do manufactured gases.

Nevertheless, the methods recommended in parts 2 and 3 can be applied, with certain restrictions and with increased uncertainty, to such gases. Although such gases may not usually be distributed to end-users, many of the applications for which calculations are required are for pressure and temperature values which fall within the ranges specified in 5.1.2.

Self-evidently, the guidelines which can be given (as well as the calculation uncertainties) become less definitive as limitations on the allowable pressure, temperature and composition ranges are relaxed.

5.2.2 Lean and rich gases

Some natural gases exist, and are distributed, which contain nitrogen, carbon dioxide, ethane or higher hydrocarbons in amounts which exceed the limits for which an uncertainty of $\pm 0,1\%$ can properly be claimed. In this context, gases which contain more than a 0,15 mole fraction of nitrogen or a 0,05 mole fraction of carbon dioxide are termed "lean", and gases which contain more than a 0,10 mole fraction of ethane or 0,035 of propane, and so on, are termed "rich".

The methods recommended in parts 2 and 3 can both be applied to these types of lean and rich gases, but with some increase in uncertainty of prediction.

For example, the method given in part 3 may be applied to give an uncertainty within $\pm 0,2\%$ for natural gases containing up to about a 0,50 mole fraction of nitrogen, 0,18 of carbon dioxide or 0,13 of ethane at pressures up to 10 MPa. A more detailed estimate of the uncertainty for each method as a function of component mole fraction is given in parts 2 and 3 where plots are given which show, for a wide range of temperatures, the pressure versus mole fraction surfaces for nitrogen, carbon dioxide, ethane and propane, respectively, with uncertainty of prediction as a parameter. The major problem in providing such plots is the paucity of high-accuracy test data.

5.2.3 Wet and sour gases

This category of gases is taken to comprise those gases which fall short of qualifying as pipeline quality natural gases only by the inclusion of undesirable components. Typically such gases may be unprocessed (well-head) or partially processed natural gases and may contain, for example, water vapour ("wet" gases), hydrogen sulfide ("sour" gases) or oxygen in amounts significantly greater than those quoted in 5.1.1, perhaps also with traces of carbonyl sulfide and process-fluid vapours such as methanol or glycols.

The method given in part 2 is applicable to any such gas, provided that the unwanted components are limited to water vapour, hydrogen sulfide and oxygen. The uncertainty of prediction is, however, substantially increased. The method given in part 3 should not be applied to such gases.

5.2.4 Manufactured gases

Manufactured gases fall into two distinct categories, as follows:

- a) those which are intended as synthetic or substitute natural gases, and which closely match true natural gases in both composition and properties;
- b) those which, whether or not intended to replace or enhance natural gas in service, do not closely match natural gases in composition.

In case (a) it is clear that, if the composition is such that the gas is indistinguishable from that of a possible true natural gas, then the methods given in parts 2 and 3 apply with no increase in uncertainty (see 5.1.5). This is, however, rarely likely to be the case. More often the manufactured gas, even if it contains inert and lower hydrocarbons in satisfactory proportions, will not exhibit the distinctive hydrocarbon "tail" of a true natural gas and may additionally contain small but significant amounts of non-alkane hydrocarbons. It is difficult to assess the effects of this upon the uncertainty of prediction.

Case (b) includes gases such as town gas, (undiluted) coke-oven gas, and LPG-air mixtures, none of which is compositionally similar to a true natural gas (even though, in the latter case, it may be operationally interchangeable with natural gas). The method given in part 3 should not be applied to any such gases. The method given in part 2 may be applied, but the uncertainty of prediction is extremely difficult to assess.

5.2.5 Summary of predictive uncertainty

The expected uncertainties of the calculation methods given in part 2 and part 3 are summarized in figure 1. The uncertainties are given as pressure versus mole fraction bar charts for various contents of nitrogen, carbon dioxide and ethane. Results are summarized for:

- a) pipeline quality natural gases within the normal ranges of temperature and pressure for transmission and distribution applications (263 K to 338 K; 0 MPa to 12 MPa);

- b) pipeline quality natural gases for the same range of temperature, but for a wider range of pressure (up to 30 MPa);
- c) wider ranges of gas composition (up to 0,5 N₂, 0,3 CO₂ and 0,2 C₂H₆) for the same ranges of temperature and pressure.

The more detailed information on which these bar charts are based is given in annex E of parts 2 and 3. Information concerning the performance outside the primary range of temperature and pressure is given in figure 1 of parts 2 and 3.

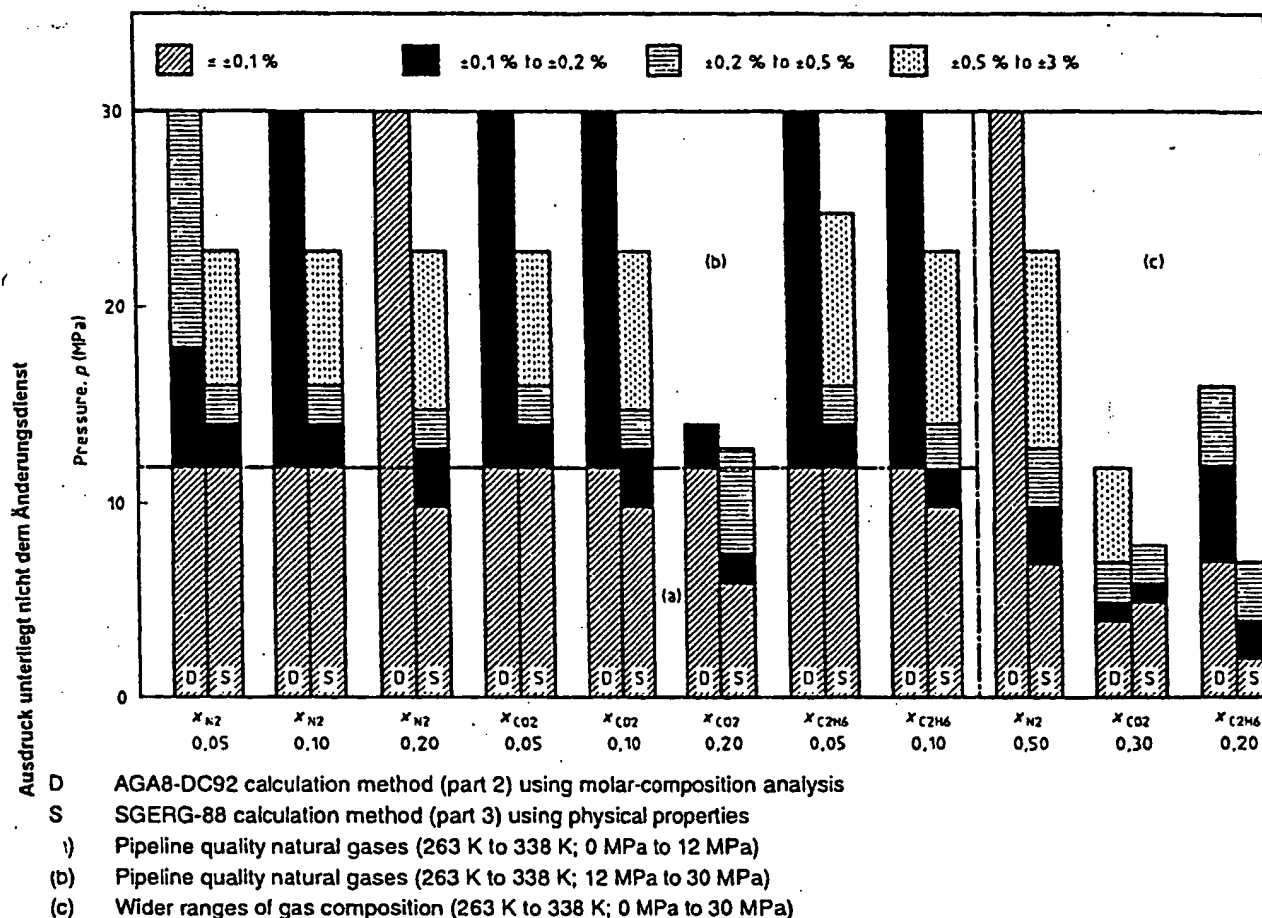


Figure 1 — Expected uncertainty of the calculation methods given in parts 2 and 3

5.2.6 Calculation of related properties

Although the express purpose of this International Standard is to permit calculations of compression factors, it is appropriate to note that other properties of natural-gas-type fluids may also be calculated by means of the methods described in parts 2 and 3. Self-evidently, the molar density ρ_m , being simply the reciprocal of the molar volume $V_m(\text{real})$, is always available from equations (1) and (2) once $Z(p, T)$ is known. The (mass) density ρ is also available, as the product of ρ_m and the mean molar mass M (molecular weight), if the latter is known, as is the case for any fluid characterized by a molar-composition analysis.

If the molar composition is not known, the mass density can instead be calculated by using the compression factors at pipeline and normal conditions together with the relative density and known mass density of dry air at normal conditions [see part 3, equation (B.42)].

Annex A (normative)

Symbols and units

| Symbol | Meaning | Value | Units |
|------------|--|------------|--|
| d | Relative density | variable | — |
| H | Molar calorific value | variable | $\text{kJ}\cdot\text{mol}^{-1}$ |
| H_S | Superior calorific value | variable | $\text{MJ}\cdot\text{m}^{-3}$ |
| M | Molar mass | variable | $\text{kg}\cdot\text{kmol}^{-1}$ |
| p | Absolute pressure | variable | kPa |
| R | Gas constant | 8,314 510 | $\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ |
| T | Absolute temperature | variable | K |
| V_m | Molar volume | variable | $\text{m}^3\cdot\text{kmol}^{-1}$ |
| x_i | Molar (mole) fraction of component i | variable | — |
| y | Set of properties | | |
| Z | Compression factor | variable | — |
| ΔZ | Uncertainty (95 % confidence limits) of predicted compression factor | variable | — |
| ρ | Mass density | variable | $\text{kg}\cdot\text{m}^{-3}$ |
| ρ_m | Molar density | V_m^{-1} | $\text{kmol}\cdot\text{m}^{-3}$ |

Annex B

(informative)

Suppliers of computer programmes

It is planned to make software available which implements this International Standard. Users are invited to contact their ISO member body or ISO Central Secretariat to enquire about the availability of such software.

Annex C (informative)

Bibliography

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INTERNATIONAL STANDARD

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12213-2

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Natural gas — Calculation of compression factor —

Part 2: Calculation using molar-composition analysis

Gaz naturel — Calcul du facteur de compression —

Partie 2: Calcul par analyse de la composition molaire

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Reference number
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Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

Draft International Standards adopted by the technical committees are circulated to the member bodies for voting. Publication as an International Standard requires approval by at least 75 % of the member bodies casting a vote.

International Standard ISO 12213-2 was prepared by Technical Committee ISO/TC 193, *Natural gas*, Subcommittee SC 1, *Analysis of natural gas*.

ISO 12213 consists of the following parts, under the general title *Natural gas — Calculation of compression factor*.

- *Part 1: Introduction and guidelines*
- *Part 2: Calculation using molar-composition analysis*
- *Part 3: Calculation using physical properties*

Annexes A to D form an integral part of this part of ISO 12213. Annexes E to G are for information only.

Natural gas — Calculation of compression factor —

Part 2: Calculation using molar-composition analysis

1 Scope

This International Standard specifies methods for the calculation of compression factors of natural gases, natural gases containing a synthetic admixture and similar mixtures at conditions under which the mixture can exist only as a gas.

This part of ISO 12213 specifies a method for the calculation of compression factors when the detailed composition of the gas by mole fractions is known, together with the relevant pressures and temperatures.

The method is applicable to pipeline quality gases within the ranges of pressure p and temperature T at which transmission and distribution operations normally take place, with an uncertainty of about $\pm 0,1$ %. It can be applied, with greater uncertainty, to wider ranges of gas composition, pressure and temperature (see annex E).

More detail concerning the scope and field of application of the method is given in part 1 of this International Standard.

2 Normative references

The following standards contain provisions which, through reference in this text, constitute provisions of this part of ISO 12213. At the time of publication, the editions indicated were valid. All standards are subject to revision, and parties to agreements based on this part of ISO 12213 are encouraged to investigate the possibility of applying the most recent editions of the standards indicated below. Members of IEC and ISO maintain registers of currently valid International Standards.

ISO 31-3:1992, *Quantities and units — Part 3: Mechanics*.

ISO 31-4:1992, *Quantities and units — Part 4: Heat*.

ISO 6976:1995, *Natural gas — Calculation of calorific values, density, relative density and Wobbe index from composition*.

ISO 12213-1:1997, *Natural gas — Calculation of compression factor — Part 1: Introduction and guidelines*.

3 Definitions

All definitions relevant to the use of this part of ISO 12213 are given in part 1.

4 Method of calculation

4.1 Principle

The method recommended uses an equation based on the concept that pipeline quality natural gas may be uniquely characterized for calculation of its volumetric properties by component analysis. This analysis, together with the pressure and temperature, are used as input data for the method.

The method uses a detailed molar-composition analysis in which all constituents present in amounts exceeding a mole fraction of 0,000 05 should be represented. Typically, this includes all alkane hydrocarbons up to about C₇ or C₈ together with nitrogen, carbon dioxide and helium.

For other gases, additional components such as water vapour, hydrogen sulfide and ethylene need to be taken into consideration (see reference [1] in annex G).

For manufactured gases, hydrogen and carbon monoxide are also likely to be significant components.

4.2 The AGA8-92DC equation

The compression factor is determined using the AGA8 detailed characterization equation (denoted hereafter as the AGA8-92DC equation). This is an extended virial-type equation. The equation is described in AGA Report No. 8(1). It may be written as

$$Z = 1 + B\rho_m - \rho_r \sum_{n=13}^{18} C_n^* + \sum_{n=13}^{58} C_n^* (b_n - c_n k_n \rho_r^{k_n}) \rho_r^{b_n} \exp(-c_n \rho_r^{k_n}) \quad \dots (1)$$

where

- Z is the compression factor;
- B is the second virial coefficient;
- ρ_m is the molar density (moles per unit volume);
- ρ_r is the reduced density;
- b_n, c_n, k_n are constants (see table B.1);
- C_n^* are coefficients which are functions of temperature and composition.

The reduced density ρ_r is related to the molar density ρ_m by the equation

$$\rho_r = K^3 \rho_m \quad \dots (2)$$

where K is a mixture size parameter.

The molar density can be written as

$$\rho_m = p/(ZRT) \quad \dots (3)$$

where

- p is the absolute pressure;
- R is the universal gas constant;
- T is the absolute temperature.

Z is calculated as follows: first the values of B and C_n^* ($n = 13$ to 58) are calculated, using relationships given in annex B. Equations (1) and (3) are then solved simultaneously for ρ_m and Z by a suitable numerical method (see figure B.1).

4.3 Input variables

The input variables required for use with the AGA8-92DC equation are the absolute pressure, absolute temperature and molar composition.

The composition is required, by mole fraction, of the following components: nitrogen, carbon dioxide, argon, methane, ethane, propane, *n*-butane, methyl-2-propane (iso-butane), *n*-pentane, methyl-2-butane (iso-pentane), hexanes, heptanes, octanes, nonanes, decanes, hydrogen, carbon monoxide, hydrogen sulfide, helium, oxygen and water.

NOTE — If the mole fractions of the heptanes, octanes, nonanes and decanes are unknown, then use of a composite C_{8+} fraction may be acceptable. The user should carry out a sensitivity analysis in order to test whether a particular approximation of this type degrades the result.

All components with mole fractions greater than 0,000 05 shall be accounted for. Trace components (such as ethylene) shall be treated as given in table 1.

If the composition is known by volume fractions, these shall be converted to mole fractions using the method given in ISO 6976. The sum of all mole fractions shall be unity to within 0,000 1.

4.4 Ranges of application

4.4.1 Pipeline quality gas

The ranges of application for pipeline quality gas are as defined below:

| | |
|--------------------------|---|
| absolute pressure | $0 \text{ MPa} \leq p \leq 12 \text{ MPa}$ |
| temperature | $263 \text{ K} \leq T \leq 338 \text{ K}$ |
| superior calorific value | $30 \text{ MJ}\cdot\text{m}^3 \leq H_S \leq 45 \text{ MJ}\cdot\text{m}^3$ |
| relative density | $0,55 \leq d \leq 0,80$ |

The mole fractions of the natural-gas components shall be within the following ranges:

| | |
|---------------------|-----------------------------------|
| methane | $0,7 \leq x_{CH_4} \leq 1,00$ |
| nitrogen | $0 \leq x_{N_2} \leq 0,20$ |
| carbon dioxide | $0 \leq x_{CO_2} \leq 0,20$ |
| ethane | $0 \leq x_{C_2H_6} \leq 0,10$ |
| propane | $0 \leq x_{C_3H_8} \leq 0,035$ |
| butanes | $0 \leq x_{C_4H_{10}} \leq 0,015$ |
| pentanes | $0 \leq x_{C_5H_{12}} \leq 0,005$ |
| hexanes | $0 \leq x_{C_6} \leq 0,001$ |
| heptanes | $0 \leq x_{C_7} \leq 0,000 5$ |
| octanes plus | $0 \leq x_{C_{8+}} \leq 0,000 5$ |
| higher hydrocarbons | |
| hydrogen | $0 \leq x_{H_2} \leq 0,10$ |
| carbon monoxide | $0 \leq x_{CO} \leq 0,03$ |
| helium | $0 \leq x_{He} \leq 0,005$ |
| water | $0 \leq x_{H_2O} \leq 0,000 15$ |

Any component for which x_i is less than 0,000 05 can be neglected.

Minor and trace components are listed in table 1.

Table 1 — Minor and trace components

| Minor or trace component | Assigned component |
|---|--------------------|
| Oxygen | oxygen |
| Argon | argon |
| Hydrogen sulfide | hydrogen sulfide |
| Ethylene, acetylene | carbon dioxide |
| Propylene, propadiene | propane |
| Butenes, butadienes | <i>n</i> -butane |
| Neo-pentane, pentenes, benzene, cyclopentane | <i>n</i> -pentane |
| All C ₆ -isomers, cyclohexane, ethylbenzene, xylenes | <i>n</i> -hexane |
| All C ₇ -isomers, cycloheptane, toluene | <i>n</i> -heptane |
| All C ₈ -isomers | <i>n</i> -octane |
| All C ₉ -isomers | <i>n</i> -nonane |
| All C ₁₀ -isomers and all higher hydrocarbons | <i>n</i> -decane |

The method applies only to mixtures in the single-phase gaseous state (above the dew point) at the conditions of temperature and pressure of interest.

4.4.2 Wider ranges of application

The ranges of application tested beyond the limits given in 4.4.1 are:

| | | |
|--------------------------|-----------------------|---------------------------------------|
| absolute pressure | 0 MPa | $\leq p \leq 65$ MPa |
| temperature | 225 K | $\leq T \leq 350$ K |
| relative density | 0,55 | $\leq d \leq 0,90$ |
| superior calorific value | 20 MJ·m ⁻³ | $\leq H_S \leq 48$ MJ·m ⁻³ |

The allowable mole fractions of the major natural gas components are:

| | |
|----------------|--------------------------------|
| methane | $0,50 \leq x_{CH_4} \leq 1,00$ |
| nitrogen | $0 \leq x_{N_2} \leq 0,50$ |
| carbon dioxide | $0 \leq x_{CO_2} \leq 0,30$ |
| ethane | $0 \leq x_{C_2H_6} \leq 0,20$ |
| propane | $0 \leq x_{C_3H_8} \leq 0,05$ |
| hydrogen | $0 \leq x_{H_2} \leq 0,10$ |

The limits for minor and trace gas components are as given in 4.4.1 for pipeline quality gas. For use of the method outside these ranges, see annex E.

4.5 Uncertainty

4.5.1 Uncertainty for pipeline quality gas

The uncertainty of results for use on all pipeline quality gas within the limits described in 4.4.1 is $\pm 0,1$ % (for the temperature range 263 K to 350 K and pressures up to 12 MPa) (see figure 1). For temperatures above 290 K and at pressures up to 30 MPa the uncertainty of the result is also $\pm 0,1$ %.

For lower temperatures, the uncertainty of $\pm 0,1$ % is at least maintained for pressures up to about 10 MPa.

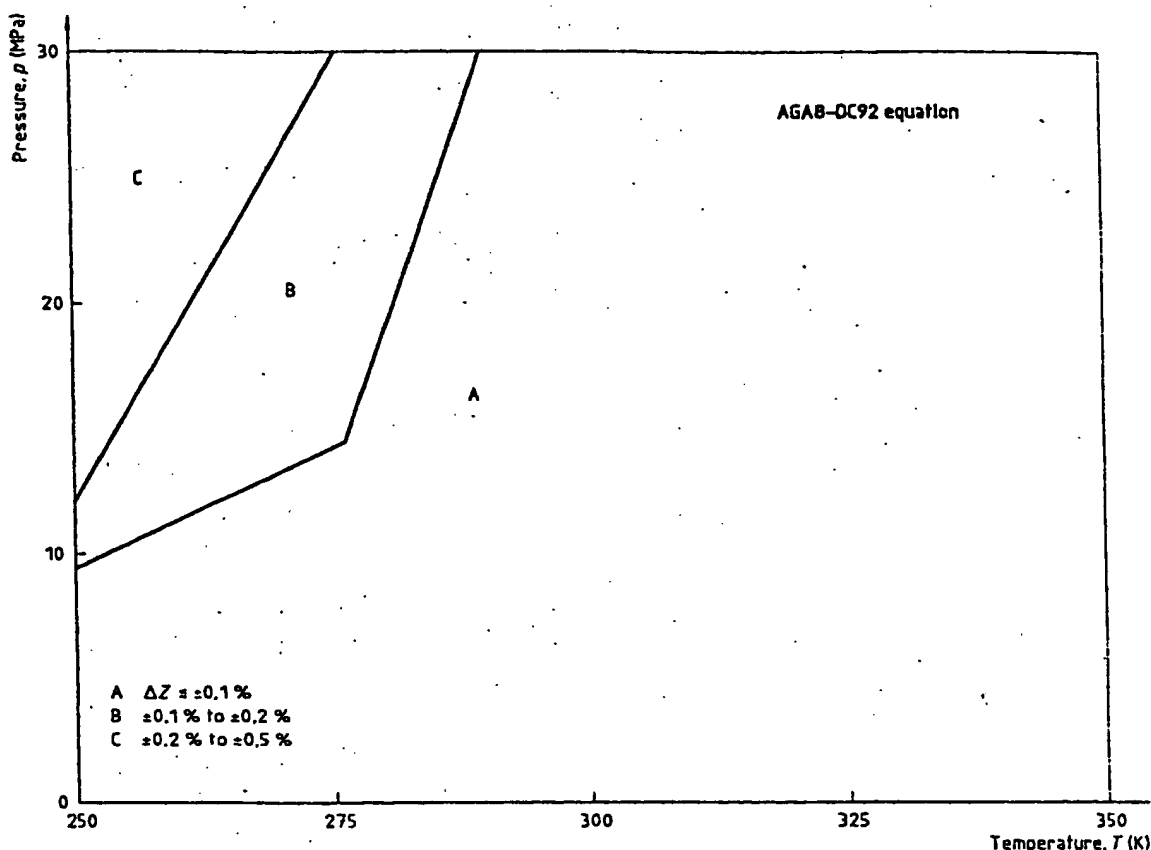


Figure 1 — Uncertainty limits for the calculation of compression factors (The uncertainty limits given are expected to be valid for natural gases and similar gases with $x_{N_2} \leq 0,20$, $x_{CO_2} \leq 0,20$, $x_{C_2H_6} \leq 0,10$ and $x_{H_2} \leq 0,10$, and for $30 \text{ MJ}\cdot\text{m}^{-3} \leq H_S \leq 45 \text{ MJ}\cdot\text{m}^{-3}$ and $0,55 \leq d \leq 0,80$)

This uncertainty level has been determined by comparison with the GERG databank of measurements of the compression factor for natural gases [2], [3]. A detailed comparison was also made with the GRI PVT data on gravimetrically prepared simulated natural-gas mixtures [4], [5].

The uncertainty of the measurements in both databanks used to test the method is of the order of $\pm 0,1 \%$.

4.5.2 Uncertainty for wider ranges of application

The estimated uncertainties for calculations of compression factors beyond the limits of quality given in 4.4.1 are discussed in annex E.

4.5.3 Impact of uncertainties of input variables

Listed in table 2 are typical values for the uncertainties of the relevant input variables. These values may be achieved under optimum operating conditions.

As a general guideline only, an error propagation analysis using the uncertainties in the input variables produces an additional uncertainty of about $\pm 0,1 \%$ in the result at 6 MPa and within the temperature range 263 K to 338 K. Above 6 MPa, the additional uncertainties are greater and increase roughly in direct proportion to the pressure.

Table 2 — Uncertainties of input variables

| Input variable | Absolute uncertainty |
|-----------------------------------|----------------------|
| Absolute pressure | $\pm 0,02$ MPa |
| Temperature | $\pm 0,15$ K |
| Mole fraction of | |
| inerts | $\pm 0,001$ |
| nitrogen | $\pm 0,001$ |
| carbon dioxide | $\pm 0,001$ |
| methane | $\pm 0,001$ |
| ethane | $\pm 0,001$ |
| propane | $\pm 0,000\ 5$ |
| butanes | $\pm 0,000\ 3$ |
| pentanes plus higher hydrocarbons | $\pm 0,000\ 1$ |
| hydrogen and carbon monoxide | $\pm 0,001$ |

4.5.4 Reporting of results.

Results for compression factor and molar density shall be reported to four and to five places of decimals, respectively, together with the pressure and temperature values and the calculation method used (ISO 12213-2, AGA8-92DC equation). For verification of calculation procedures, it is useful to carry extra digits.

5 Suppliers of computer programmes

It is planned to make software available which implements this International Standard. Users are invited to contact their ISO member body or ISO Central Secretariat to enquire about the availability of such software.

Annex A (normative)

Symbols and units

| Symbol | Meaning | Units |
|-------------|---|---|
| a_n | Constant in table B.1 | — |
| B | Second virial coefficient | $\text{m}^3 \cdot \text{kmol}^{-1}$ |
| B_{nij}^* | Mixture interaction coefficient [equations (B.1) and (B.2)] | — |
| B_n | Constant in table B.1 | — |
| c_n | Constant in table B.1 | — |
| C_n^* | Coefficients which are functions of temperature and composition | — |
| E_i | Characteristic energy parameter for i th component (table B.2) | K |
| E_j | Characteristic energy parameter for j th component (table B.2) | K |
| E_{ij} | Binary energy parameter for second virial coefficient | K |
| E_{ij}^* | Binary energy interaction parameter for second virial coefficient (table B.3) | — |
| F | Mixture high-temperature parameter | — |
| F_i | High-temperature parameter for i th component (table B.2) | — |
| F_j | High-temperature parameter for j th component (table B.2) | — |
| f_n | Constant in table B.1 | — |
| G | Mixture orientation parameter | — |
| G_i | Orientation parameter for i th component (table B.2) | — |
| G_j | Orientation parameter for j th component (table B.2) | — |
| G_{ij} | Binary orientation parameter | — |
| G_{ij}^* | Binary interaction parameter for orientation (table B.2) | — |
| g_n | Constant in table B.1 | — |
| H_S | Superior calorific value | $\text{MJ} \cdot \text{m}^3$ |
| K | Size parameter | $(\text{m}^3/\text{kmol})^{1/3}$ |
| K_i | Size parameter for i th component (table B.2) | $(\text{m}^3/\text{kmol})^{1/3}$ |
| K_j | Size parameter for j th component (table B.2) | $(\text{m}^3/\text{kmol})^{1/3}$ |
| K_{ij} | Binary interaction parameter for size (table B.3) | — |
| k_n | Constant in table B.1 | — |
| M | Molar mass | $\text{kg} \cdot \text{kmol}^{-1}$ |
| M_i | Molar mass of i th component | $\text{kg} \cdot \text{kmol}^{-1}$ |
| N | Number of components in gas mixture | — |
| n | An integer (from 1 to 58) | — |
| p | Absolute pressure | MPa |
| Q | Quadrupole parameter | — |
| Q_i | Quadrupole parameter for i th component | — |
| Q_j | Quadrupole parameter for j th component | — |
| q_n | Constant (table B.1) | — |
| R | Gas constant (= 0,008 314 510) | $\text{MJ} \cdot (\text{kmol} \cdot \text{K})^{-1}$ |
| S_i | Dipole parameter for i th component (table B.2) | — |
| S_j | Dipole parameter for j th component (table B.2) | — |
| s_n | Constant (table B.1) | — |

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| Symbol | Meaning | Units |
|----------|---|----------------------|
| T | Absolute temperature | K |
| U | Mixture energy parameter | K |
| U_{ij} | Binary interaction parameter for mixture energy (table B.3) | — |
| u_n | Constant in table B.1 | — |
| w_i | Association parameter for i th component (table B.2) | — |
| w_j | Association parameter for j th component (table B.2) | — |
| w_n | Constant (table B.1) | — |
| x_i | Mole fraction of i th component in gas mixture | — |
| x_j | Mole fraction of j th component in gas mixture | — |
| Z | Compression factor | — |
| ρ | Mass density | kg·m ⁻³ |
| ρ_r | Reduced density of gas | — |
| ρ_m | Molar density | kmol·m ⁻³ |

Annex B (normative)

Description of the AGA8-92DC method

B.1 General

For gas mixtures, the compression factor Z is calculated using the equations given in 4.2. This annex gives a detailed description of the computations and the necessary numerical values. The description is based upon that given in AGA Report No. 8 [1]. A programme implementing this description is given in annex F, and as such provides the correct solution. Other computational procedures are acceptable provided that they can be demonstrated to yield identical numerical results (see annex C for examples).

B.2 Computer implementation of the AGA8-92DC method

B.2.1 Overview of the calculation procedure

- I Input the absolute temperature T , absolute pressure p and mole fraction of each component x_i of the mixture.
NOTE — For pressure and temperature, values known in any other units will first have to be converted precisely to values in megapascals and kelvins, respectively (see ISO 31-3 and ISO 31-4 and annex D for relevant conversion factors).
- II Compute the equation of state coefficients B and C_n^* ($n = 13$ to 58) that depend on T and x_i .
- III Solve iteratively for the molar density ρ_m , using the equation of state rearranged to give the pressure p .
- IV Output the compression factor after the computed pressure from step III and the input pressure from step I agree within a specified range of convergence (e.g. $1E-06$).

Figure B.1 shows a flow diagram of these steps.

B.2.2 Details of the calculation procedure

Step I

Input the absolute temperature T , absolute pressure p and mole fraction x_i of each constituent in the natural-gas mixture.

Step II

At the absolute temperature T and the mole fractions x_i of the natural gas (as input from step I), compute the composition- and temperature-dependent coefficients B and C_n^* ($n = 13$ to 58).

The second virial coefficient B is given by the following equations:

$$B = \sum_{n=1}^{18} a_n T^{-u_n} \sum_{i=1}^N \sum_{j=1}^N x_i x_j B_{nij}^* E_{ij}^{u_n} (K_i K_j)^{3/2} \quad \dots (B.1)$$

$$B_{nij}^* = (G_{ij} + 1 - g_n)^{r_n} (Q_i Q_j + 1 - q_n)^{q_n} (F_i^{1/2} F_j^{1/2} + 1 - f_n)^{f_n} (S_i S_j + 1 - s_n)^{s_n} (W_i W_j + 1 - w_n)^{w_n} \quad \dots (B.2)$$

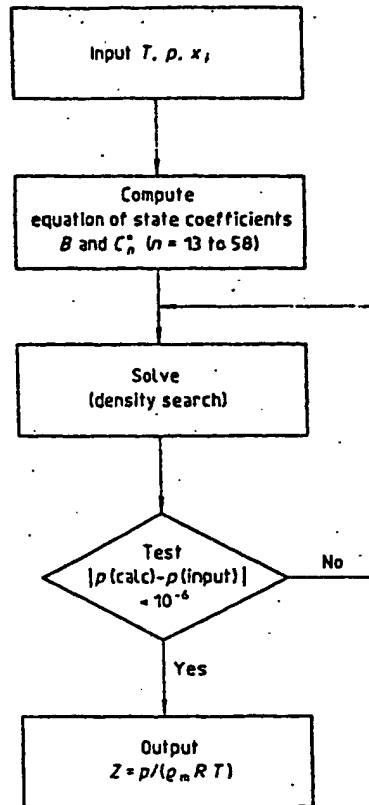


Figure B.1 — AGA8-92DC equation — Calculation flow diagram

The binary parameters E_{ij} and G_{ij} are calculated using the following equations:

$$E_{ij} = E_{ij}^* (E_i E_j)^{1/2} \quad \dots (B.3)$$

$$G_{ij} = G_{ij}^* (G_i + G_j)/2 \quad \dots (B.4)$$

Note that all values of the binary interaction parameters E_{ij}^* and G_{ij}^* are 1,0 except for the values given in table B.3.

The coefficients C_n^* ($n = 13$ to 58) are given by the equation:

$$C_n^* = a_n (G + 1 - g_n)^{g_n} (Q^2 + 1 - q_n)^{q_n} (F + 1 - f_n)^{f_n} U^{u_n} T^{-u_n} \quad \dots (B.5)$$

The mixture parameters U , G and Q are calculated using the following conformal solution mixing equations, where in the double sums i ranges from 1 to $N - 1$ and, for each value of i , j ranges from $i + 1$ to N :

$$U^5 = \left(\sum_{i=1}^N x_i E_i^{5/2} \right)^2 + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^N x_i x_j (U_{ij}^5 - 1) (E_i E_j)^{5/2} \quad \dots (B.6)$$

$$G = \sum_{i=1}^N x_i G_i + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^N x_i x_j (G_{ij}^* - 1) (G_i + G_j) \quad \dots (B.7)$$

$$Q = \sum_{i=1}^N x_i Q_i \quad \dots (B.8)$$

$$F = \sum_{i=1}^N x_i^2 F_i \quad \dots (B.9)$$

It should be noted that all values of the binary interaction parameters K_{ij} , E_{ij}^* , G_{ij}^* and U_{ij} are 1,0 except for the values given in table B.3. Also note that F_i is zero for all components except hydrogen, for which $F(\text{H}_2) = 1,0$, and that W_i is zero for all components except water, for which $W(\text{H}_2\text{O}) = 1,0$.

Step III

In the computation of the compression factor Z , the composition of the gas is known, the absolute temperature T of the gas is known and the absolute pressure is known. The problem then is to compute the molar density ρ_m , using the equation of state expression for the pressure p . For this purpose, the definition of the compression factor Z as given in equation (1) (see 4.2) is substituted into equation (3) to obtain an equation for the pressure as given in equation (B.10):

$$p = \rho_m RT \left[1 + B \rho_m - \rho_r \sum_{n=13}^{18} C_n^* + \sum_{n=13}^{58} C_n^* (b_n - c_n k_n \rho_r^{k_n}) \rho_r^{b_n} \exp(-c_n \rho_r^{k_n}) \right] \quad \dots (B.10)$$

Equation (B.10) is solved using standard equation of state density search algorithms. Having obtained an equation for the pressure p [equation (B.10)], the problem is then to search for the value of the molar density ρ_m that will yield the pressure that is within a preset limit (e.g. 1×10^{-6}) equal to the input pressure.

The reduced density ρ_r is related to the molar density ρ_m by the mixture size parameter [see equation (2) in 4.2].

The mixture size parameter K is calculated using the following equation:

$$K^5 = \left(\sum_{i=1}^N x_i K_i^{5/2} \right)^2 + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^N x_i x_j (K_{ij}^5 - 1) (K_i K_j)^{5/2} \quad \dots (B.11)$$

Note that in the summations the subscript i refers to the i th component in the gas mixture and the subscript j refers to the j th component in the gas mixture. The quantity N is the number of components in the mixture. Thus, in the single summation, i ranges over the integer values from 1 to N . For example, for a mixture of 12 components, $N = 12$ and there would be 12 terms in the single sum. In the double summation, i ranges from 1 to $N - 1$ and, for each value of i , j ranges from $i + 1$ to N . For example, for a mixture of 12 components, there would be 66 terms in the double summation if all values of K_{ij} differed from 1,0. However, because many of the values of K_{ij} are 1,0, the number of non-zero terms in the double summation is small for many natural-gas mixtures. Note that all values of K_{ij} are 1,0 except for the values given in table B.3.

Step IV

Once the molar density ρ_m has been obtained in step III, the compression factor is calculated in step IV using the pressure, temperature, molar density and gas constant:

$$Z = p / (\rho_m RT) \quad \dots (B.12)$$

NOTE — The density ρ (mass per unit volume) can be calculated as follows:

$$\rho = M \rho_m \quad \dots (B.13)$$

where M is calculated from the equation:

$$M = \sum_{i=1}^N x_i M_i$$

... (B.14)

Report the density to three places of decimals.

Table B.1 — Equation of state parameters

| n | a_n | b_n | c_n | k_n | u_n | g_n | q_n | f_n | s_n | w_n |
|-----|-------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 1 | 0,153 832 600 | 1 | 0 | 0 | 0,0 | 0 | 0 | 0 | 0 | 0 |
| 2 | 1,341 953 000 | 1 | 0 | 0 | 0,5 | 0 | 0 | 0 | 0 | 0 |
| 3 | -2,998 583 000 | 1 | 0 | 0 | 1,0 | 0 | 0 | 0 | 0 | 0 |
| 4 | -0,048 312 280 | 1 | 0 | 0 | 3,5 | 0 | 0 | 0 | 0 | 0 |
| 5 | 0,375 796 500 | 1 | 0 | 0 | -0,5 | 1 | 0 | 0 | 0 | 0 |
| 6 | -1,589 575 000 | 1 | 0 | 0 | 4,5 | 1 | 0 | 0 | 0 | 0 |
| 7 | -0,053 588 470 | 1 | 0 | 0 | 0,5 | 0 | 1 | 0 | 0 | 0 |
| 8 | 0,886 594 630 | 1 | 0 | 0 | 7,5 | 0 | 0 | 0 | 1 | 0 |
| 9 | -0,710 237 040 | 1 | 0 | 0 | 9,5 | 0 | 0 | 0 | 1 | 0 |
| 10 | -1,471 722 000 | 1 | 0 | 0 | 6,0 | 0 | 0 | 0 | 0 | 1 |
| 11 | 1,321 850 350 | 1 | 0 | 0 | 12,0 | 0 | 0 | 0 | 0 | 1 |
| 12 | -0,786 659 250 | 1 | 0 | 0 | 12,5 | 0 | 0 | 0 | 0 | 1 |
| 13 | 2,291 290 × 10 ⁻⁹ | 1 | 1 | 3 | -6,0 | 0 | 0 | 1 | 0 | 1 |
| 14 | 0,157 672 400 | 1 | 1 | 2 | 2,0 | 0 | 0 | 0 | 0 | 0 |
| 15 | -0,436 386 400 | 1 | 1 | 2 | 3,0 | 0 | 0 | 0 | 0 | 0 |
| 16 | -0,044 081 590 | 1 | 1 | 2 | 2,0 | 0 | 1 | 0 | 0 | 0 |
| 17 | -0,003 433 888 | 1 | 1 | 4 | 2,0 | 0 | 0 | 0 | 0 | 0 |
| 18 | 0,032 059 050 | 1 | 1 | 4 | 11,0 | 0 | 0 | 0 | 0 | 0 |
| 19 | 0,024 873 550 | 2 | 0 | 0 | -0,5 | 0 | 0 | 0 | 0 | 0 |
| 20 | 0,073 322 790 | 2 | 0 | 0 | 0,5 | 0 | 0 | 0 | 0 | 0 |
| 21 | -0,001 600 573 | 2 | 1 | 2 | 0,0 | 0 | 0 | 0 | 0 | 0 |
| 22 | 0,642 470 600 | 2 | 1 | 2 | 4,0 | 0 | 0 | 0 | 0 | 0 |
| 23 | -0,416 260 100 | 2 | 1 | 2 | 6,0 | 0 | 0 | 0 | 0 | 0 |
| 24 | -0,066 899 570 | 2 | 1 | 4 | 21,0 | 0 | 0 | 0 | 0 | 0 |
| 25 | 0,279 179 500 | 2 | 1 | 4 | 23,0 | 1 | 0 | 0 | 0 | 0 |
| 26 | -0,696 605 100 | 2 | 1 | 4 | 22,0 | 0 | 1 | 0 | 0 | 0 |
| 27 | -0,002 860 589 | 2 | 1 | 4 | -1,0 | 0 | 0 | 1 | 0 | 0 |
| 28 | -0,008 098 836 | 3 | 0 | 0 | -0,5 | 0 | 1 | 0 | 0 | 0 |
| 29 | 3,150 547 000 | 3 | 1 | 1 | 7,0 | 1 | 0 | 0 | 0 | 0 |
| 30 | 0,007 224 479 | 3 | 1 | 1 | -1,0 | 0 | 0 | 1 | 0 | 0 |
| 31 | -0,705 752 900 | 3 | 1 | 2 | 6,0 | 0 | 0 | 0 | 0 | 0 |
| 32 | 0,534 979 200 | 3 | 1 | 2 | 4,0 | 1 | 0 | 0 | 0 | 0 |
| 33 | -0,079 314 910 | 3 | 1 | 3 | 1,0 | 1 | 0 | 0 | 0 | 0 |
| 34 | -1,418 465 000 | 3 | 1 | 3 | 9,0 | 1 | 0 | 0 | 0 | 0 |
| 35 | -5,999 05 × 10 ⁻¹⁷ | 3 | 1 | 4 | -13,0 | 0 | 0 | 1 | 0 | 0 |
| 36 | 0,105 840 200 | 3 | 1 | 4 | 21,0 | 0 | 0 | 0 | 0 | 0 |
| 37 | 0,034 317 290 | 3 | 1 | 4 | 8,0 | 0 | 1 | 0 | 0 | 0 |
| 38 | -0,007 022 847 | 4 | 0 | 0 | -0,5 | 0 | 0 | 0 | 0 | 0 |
| 39 | 0,024 955 870 | 4 | 0 | 0 | 0,0 | 0 | 0 | 0 | 0 | 0 |
| 40 | 0,042 968 180 | 4 | 1 | 2 | 2,0 | 0 | 0 | 0 | 0 | 0 |
| 41 | 0,746 545 300 | 4 | 1 | 2 | 7,0 | 0 | 0 | 0 | 0 | 0 |
| 42 | -0,291 961 300 | 4 | 1 | 2 | 9,0 | 0 | 1 | 0 | 0 | 0 |
| 43 | 7,294 616 000 | 4 | 1 | 4 | 22,0 | 0 | 0 | 0 | 0 | 0 |
| 44 | -9,936 757 000 | 4 | 1 | 4 | 23,0 | 0 | 0 | 0 | 0 | 0 |
| 45 | -0,005 399 808 | 5 | 0 | 0 | 1,0 | 0 | 0 | 0 | 0 | 0 |
| 46 | -0,243 256 700 | 5 | 1 | 2 | 9,0 | 0 | 0 | 0 | 0 | 0 |
| 47 | 0,049 870 160 | 5 | 1 | 2 | 3,0 | 0 | 1 | 0 | 0 | 0 |
| 48 | 0,003 733 797 | 5 | 1 | 4 | 8,0 | 0 | 0 | 0 | 0 | 0 |
| 49 | 1,874 951 000 | 5 | 1 | 4 | 23,0 | 0 | 1 | 0 | 0 | 0 |
| 50 | 0,002 168 144 | 6 | 0 | 0 | 1,5 | 0 | 0 | 0 | 0 | 0 |
| 51 | -0,658 716 400 | 6 | 1 | 2 | 5,0 | 1 | 0 | 0 | 0 | 0 |
| 52 | 0,000 205 518 | 7 | 0 | 0 | -0,5 | 0 | 1 | 0 | 0 | 0 |
| 53 | 0,009 776 195 | 7 | 1 | 2 | 4,0 | 0 | 0 | 0 | 0 | 0 |
| 54 | -0,020 487 080 | 8 | 1 | 1 | 7,0 | 1 | 0 | 0 | 0 | 0 |
| 55 | 0,015 573 220 | 8 | 1 | 2 | 3,0 | 0 | 0 | 0 | 0 | 0 |
| 56 | 0,006 862 415 | 8 | 1 | 2 | 0,0 | 1 | 0 | 0 | 0 | 0 |
| 57 | -0,001 226 752 | 9 | 1 | 2 | 1,0 | 0 | 0 | 0 | 0 | 0 |
| 58 | 0,002 850 908 | 9 | 1 | 2 | 0,0 | 0 | 1 | 0 | 0 | 0 |

Table B.2 — Characterization parameters

| Identifi- cation number | Compound | Molar mass | Energy parameter | Size parameter | Orientation parameter | Quadrupole parameter | High- temp. param- eter | Dipole parameter | Associ- ation param- eter |
|-------------------------------|------------------|--------------------------------|---------------------|--|--------------------------|-------------------------|----------------------------------|---------------------|------------------------------------|
| | | M_i kg·kmol ⁻¹ | E_i K | K_i (m ³ /kmol) ^{1/3} | C_i | Q_i | F_i | S_i | W_i |
| 1 | Methane | 16,043 0 | 151,318 300 | 0,461 925 5 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 |
| 2 | Nitrogen | 28,013 5 | 99,737 780 | 0,447 915 3 | 0,027 815 | 0,0 | 0,0 | 0,0 | 0,0 |
| 3 | Carbon dioxide | 44,010 0 | 241,960 600 | 0,455 748 9 | 0,189 065 | 0,690 000 | 0,0 | 0,0 | 0,0 |
| 4 | Ethane | 30,070 0 | 244,166 700 | 0,527 920 9 | 0,079 300 | 0,0 | 0,0 | 0,0 | 0,0 |
| 5 | Propane | 44,097 0 | 298,118 300 | 0,583 749 0 | 0,141 239 | 0,0 | 0,0 | 0,0 | 0,0 |
| 6 | Water | 18,015 3 | 514,015 600 | 0,382 586 8 | 0,332 500 | 1,067 750 | 0,0 | 1,582 200 | 1,0 |
| 7 | Hydrogen sulfide | 34,082 0 | 296,355 000 | 0,461 826 3 | 0,088 500 | 0,633 276 | 0,0 | 0,390 000 | 0,0 |
| 8 | Hydrogen | 2,015 9 | 26,957 940 | 0,351 491 6 | 0,034 369 | 0,0 | 1,0 | 0,0 | 0,0 |
| 9 | Carbon monoxide | 28,010 0 | 105,534 800 | 0,453 389 4 | 0,038 953 | 0,0 | 0,0 | 0,0 | 0,0 |
| 10 | Oxygen | 31,998 8 | 122,766 700 | 0,418 695 4 | 0,021 000 | 0,0 | 0,0 | 0,0 | 0,0 |
| 11 | iso-Butane | 58,123 0 | 324,068 900 | 0,640 693 7 | 0,256 692 | 0,0 | 0,0 | 0,0 | 0,0 |
| 12 | n-Butane | 58,123 0 | 337,638 900 | 0,634 142 3 | 0,281 835 | 0,0 | 0,0 | 0,0 | 0,0 |
| 13 | iso-Pentane | 72,150 0 | 365,599 900 | 0,673 857 7 | 0,332 267 | 0,0 | 0,0 | 0,0 | 0,0 |
| 14 | n-Pentane | 72,150 0 | 370,682 300 | 0,679 830 7 | 0,366 911 | 0,0 | 0,0 | 0,0 | 0,0 |
| 15 | n-Hexane | 86,177 0 | 402,636 293 | 0,717 511 8 | 0,289 731 | 0,0 | 0,0 | 0,0 | 0,0 |
| 16 | n-Heptane | 100,204 0 | 427,722 630 | 0,752 518 9 | 0,337 542 | 0,0 | 0,0 | 0,0 | 0,0 |
| 17 | n-Octane | 114,231 0 | 450,325 022 | 0,784 955 0 | 0,383 381 | 0,0 | 0,0 | 0,0 | 0,0 |
| 18 | n-Nonane | 128,258 0 | 470,840 891 | 0,815 273 1 | 0,427 354 | 0,0 | 0,0 | 0,0 | 0,0 |
| 19 | n-Decane | 142,285 0 | 489,558 373 | 0,843 782 6 | 0,469 659 | 0,0 | 0,0 | 0,0 | 0,0 |
| 20 | Helium | 4,002 6 | 2,610 111 | 0,358 988 8 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 |
| 21 | Argon | 39,948 0 | 119,629 900 | 0,421 655 1 | 0,0 | 0,0 | 0,0 | 0,0 | 0,0 |

Table B.3 — Binary interaction parameter values

| Identification number | | Component pair | E_{ij}^* | U_{ij} | K_{ij} | G_{ij}^* |
|-----------------------|-----|--------------------|------------|-----------|-----------|------------|
| i | j | | | | | |
| 1 | 2 | Methane + nitrogen | 0,971 640 | 0,886 106 | 1,003 630 | 0,807 653 |
| | 3 | carbon dioxide | 0,960 644 | 0,963 827 | 0,995 933 | |
| | 4 | ethane | | | | |
| | 5 | propane | 0,994 635 | 0,990 877 | 1,007 619 | |
| | 6 | water | 0,708 218 | | | |
| | 7 | hydrogen sulfide | 0,931 484 | 0,736 833 | 1,000 080 | |
| | 8 | hydrogen | 1,170 520 | 1,156 390 | 1,023 260 | |
| | 9 | carbon monoxide | 0,990 126 | | | |
| | 10 | oxygen | | | | |
| | 11 | iso-butane | 1,019 530 | | | |
| | 12 | <i>n</i> -butane | 0,989 844 | 0,992 291 | 0,997 596 | |
| | 13 | iso-pentane | 1,002 350 | | | |
| | 14 | <i>n</i> -pentane | 0,999 268 | 1,003 670 | 1,002 529 | |
| | 15 | <i>n</i> -hexane | 1,107 274 | 1,302 576 | 0,982 962 | |
| | 16 | <i>n</i> -heptane | 0,880 880 | 1,191 904 | 0,983 565 | |
| | 17 | <i>n</i> -octane | 0,880 973 | 1,205 769 | 0,982 707 | |
| | 18 | <i>n</i> -nonane | 0,881 067 | 1,219 634 | 0,981 849 | |
| | 19 | <i>n</i> -decane | 0,881 161 | 1,233 498 | 0,980 991 | |

| Identification number | | Component pair | E_{ij}^* | U_{ij} | K_{ij} | G_{ij}^* |
|-----------------------|-----|-------------------------------------|------------|-----------|-----------|------------|
| i | j | | | | | |
| 2 | 3 | Nitrogen + carbon dioxide | 1,022 740 | | | |
| | 4 | ethane | 0,970 120 | 0,835 058 | 0,982 361 | 0,982 746 |
| | 5 | propane | 0,945 939 | 0,816 431 | 1,007 960 | |
| | 6 | water | 0,746 954 | 0,915 502 | | |
| | 7 | hydrogen sulfide | 0,902 271 | | | |
| | 8 | hydrogen | 1,086 320 | 0,993 476 | 0,942 596 | |
| | 9 | carbon monoxide | 1,005 710 | 0,408 838 | 1,032 270 | |
| | 10 | oxygen | 1,021 000 | | | |
| | 11 | iso-butane | 0,946 914 | | | |
| | 12 | <i>n</i> -butane | 0,973 384 | 0,993 556 | | |
| | 13 | iso-pentane | 0,959 340 | | | |
| | 14 | <i>n</i> -pentane | 0,945 520 | | | |
| 3 | 4 | Carbon dioxide + ethane | 0,925 053 | 0,969 870 | 1,008 510 | 0,370 296 |
| | 5 | propane | 0,960 237 | | | |
| | 6 | water | 0,849 408 | | | |
| | 7 | hydrogen sulfide | 0,955 052 | | | 1,673 090 |
| | 8 | hydrogen | 1,281 790 | 1,045 290 | 1,007 790 | |
| | 9 | carbon monoxide | 1,500 000 | | | |
| | 10 | oxygen | | 0,900 000 | | |
| | 11 | iso-butane | 0,906 849 | | | |
| | 12 | <i>n</i> -butane | 0,897 362 | | | |
| | 13 | iso-pentane | 0,726 255 | | | |
| | 14 | <i>n</i> -pentane | 0,859 764 | | | |
| | 15 | <i>n</i> -hexane | 0,855 134 | 1,066 638 | 0,910 183 | |
| | 16 | <i>n</i> -heptane | 0,831 229 | 1,077 634 | 0,895 362 | |
| | 17 | <i>n</i> -octane | 0,808 310 | 1,088 178 | 0,881 152 | |
| 4 | 18 | <i>n</i> -nonane | 0,786 323 | 1,098 291 | 0,867 520 | |
| | 19 | <i>n</i> -decane | 0,765 171 | 1,108 021 | 0,854 406 | |
| | 5 | Ethane + propane | 1,022 560 | 1,065 173 | 0,986 893 | |
| | 6 | water | 0,693 168 | | | |
| | 7 | hydrogen sulfide | 0,946 871 | 0,971 926 | 0,999 969 | |
| | 8 | hydrogen | 1,164 460 | 1,616 660 | 1,020 340 | |
| | 9 | carbon monoxide | | | | |
| | 10 | oxygen | | | | |
| | 11 | iso-butane | | 1,250 000 | | |
| | 12 | <i>n</i> -butane | 1,013 060 | 1,250 000 | | |
| | 13 | iso-pentane | | 1,250 000 | | |
| | 14 | <i>n</i> -pentane | 1,005 320 | 1,250 000 | | |
| | 5 | Propane + hydrogen | 1,034 787 | | | |
| | 12 | <i>n</i> -butane | 1,004 900 | | | |
| 7 | 15 | Hydrogen sulfide + <i>n</i> -hexane | 1,008 692 | 1,028 973 | 0,968 130 | |
| | 16 | <i>n</i> -heptane | 1,010 126 | 1,033 754 | 0,962 870 | |
| | 17 | <i>n</i> -octane | 1,011 501 | 1,038 338 | 0,957 828 | |
| | 18 | <i>n</i> -nonane | 1,012 821 | 1,042 735 | 0,952 441 | |
| | 19 | <i>n</i> -decane | 1,014 089 | 1,046 966 | 0,948 338 | |
| 8 | 9 | Hydrogen + carbon monoxide | 1,100 000 | | | |
| | 10 | oxygen | | | | |
| | 11 | iso-butane | 1,300 000 | | | |
| | 12 | <i>n</i> -butane | 1,300 000 | | | |

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Annex C (normative)

Example calculations

The following example calculations have been carried out using the validated computer programme described in reference [1], which incorporates the subroutine described in annex B.

Table C.1 — Gas analysis in mole fractions

| | Gas 1 | Gas 2 | Gas 3 | Gas 4 | Gas 5 | Gas 6 |
|-----------------------------------|---------|---------|---------|---------|---------|---------|
| x_{CO_2} | 0,006 | 0,005 | 0,015 | 0,016 | 0,076 | 0,011 |
| x_{N_2} | 0,003 | 0,031 | 0,010 | 0,100 | 0,057 | 0,117 |
| x_{H_2} | 0,00 | 0,00 | 0,00 | 0,095 | 0,00 | 0,00 |
| x_{CO} | 0,00 | 0,00 | 0,00 | 0,010 | 0,00 | 0,00 |
| x_{CH_4} | 0,965 | 0,907 | 0,859 | 0,735 | 0,812 | 0,826 |
| $x_{\text{C}_2\text{H}_6}$ | 0,018 | 0,045 0 | 0,085 | 0,033 | 0,043 | 0,035 |
| $x_{\text{C}_3\text{H}_8}$ | 0,004 5 | 0,008 4 | 0,023 | 0,007 4 | 0,009 | 0,007 5 |
| $x_{\text{iso-C}_4\text{H}_{10}}$ | 0,001 0 | 0,001 0 | 0,003 5 | 0,001 2 | 0,001 5 | 0,001 2 |
| $x_{n\text{-C}_4\text{H}_{10}}$ | 0,001 0 | 0,001 5 | 0,003 5 | 0,001 2 | 0,001 5 | 0,001 2 |
| $x_{\text{iso-C}_5\text{H}_{12}}$ | 0,000 5 | 0,000 3 | 0,000 5 | 0,000 4 | 0,00 | 0,000 4 |
| $x_{n\text{-C}_5\text{H}_{12}}$ | 0,000 3 | 0,000 4 | 0,000 5 | 0,000 4 | 0,00 | 0,000 4 |
| $x_{\text{C}_6\text{H}_{14}}$ | 0,000 7 | 0,000 4 | 0,00 | 0,000 2 | 0,00 | 0,000 2 |
| $x_{\text{C}_7\text{H}_{16}}$ | 0,00 | 0,00 | 0,00 | 0,000 1 | 0,00 | 0,000 1 |
| $x_{\text{C}_8\text{H}_{18}}$ | 0,00 | 0,00 | 0,00 | 0,000 1 | 0,00 | 0,00 |

Table C.2 — Results (Z-values)

| Conditions | | Gas 1 | Gas 2 | Gas 3 | Gas 4 | Gas 5 | Gas 6 |
|------------|-----------|----------|----------|----------|----------|----------|----------|
| p bar | t °C | | | | | | |
| 60 | - 3,15 | 0,840 53 | 0,833 48 | 0,793 80 | 0,885 50 | 0,826 09 | 0,853 80 |
| 60 | 6,85 | 0,861 99 | 0,855 96 | 0,822 06 | 0,901 44 | 0,849 69 | 0,873 70 |
| 60 | 16,85 | 0,880 06 | 0,874 84 | 0,845 44 | 0,915 01 | 0,869 44 | 0,890 52 |
| 60 | 36,85 | 0,908 67 | 0,904 46 | 0,881 83 | 0,936 74 | 0,900 52 | 0,917 23 |
| 60 | 56,85 | 0,930 11 | 0,926 96 | 0,908 68 | 0,953 18 | 0,923 68 | 0,937 30 |
| 120 | - 3,15 | 0,721 33 | 0,710 44 | 0,641 45 | 0,810 24 | 0,695 40 | 0,750 74 |
| 120 | 6,85 | 0,760 25 | 0,750 66 | 0,689 71 | 0,837 82 | 0,737 80 | 0,785 86 |
| 120 | 16,85 | 0,793 17 | 0,784 75 | 0,731 23 | 0,861 37 | 0,773 69 | 0,815 69 |
| 120 | 36,85 | 0,845 15 | 0,838 63 | 0,796 98 | 0,899 13 | 0,830 22 | 0,863 11 |
| 120 | 56,85 | 0,883 83 | 0,878 70 | 0,845 53 | 0,927 66 | 0,872 11 | 0,898 62 |

Annex D (normative)

Pressure and temperature conversion factors

If the input variables pressure and temperature are not in the necessary units of megapascals and kelvins, then conversions will have to be made in order to use the Fortran implementation. A selection of appropriate conversion factors is given below:

Pressure

$$p \text{ (MPa)} = [p(\text{bar})] \times 10^{-1}$$

$$p \text{ (MPa)} = [p(\text{atm})] \times 0,101\,325$$

$$p \text{ (MPa)} = [p(\text{psia})]/145,038$$

$$p \text{ (MPa)} = [p(\text{psig}) + 14,695\,9]/145,038$$

Temperature

$$T \text{ (K)} = t(^{\circ}\text{C}) + 273,15$$

$$T \text{ (K)} = [t(^{\circ}\text{F}) - 32]/1,8 + 273,15$$

$$T \text{ (K)} = [t(^{\circ}\text{R})]/1,8$$

Annex E (informative)

Performance over wider ranges of application

The AGA8-92DC equation has been comprehensively tested, over the temperature range 263 K to 338 K and at pressures up to 30 MPa, with the GERG data [2], [3] and the Gas Research Institute data [4] for gases within the ranges of composition given for pipeline quality gases (see 4.4.1). Within these limits, the uncertainties are as given in 4.5.

Rough estimates of the uncertainties involved in calculations of compression factors for wider ranges of application (with respect to composition) (see 4.4.2) are plotted in figures E.1 to E.4 as pressure-composition plots for nitrogen, carbon dioxide, ethane and propane, respectively.

In figures E.1 to E.4 the performance of the AGA8-92DC method is illustrated up to a maximum pressure of 30 MPa. The uncertainty limits are dependent upon pressure, temperature and composition, and are also strongly affected by the proximity of the phase boundary. The estimated uncertainty limits presented below are based upon less comprehensive data, published as a supplement to the GERG databank [3], and upon the databanks in references [2] and [4]. Reference [4] also provides data up to 70 MPa. The uncertainty limits given in figures E.1 to E.4 are always for the worst-case result, i.e. they are the least optimistic choice.

Dashed lines are used to separate two regions of estimated uncertainty when the experimental evidence is not sufficient to determine the position of the boundary. The detailed composition of the gas will have a strong influence on the position of the phase boundary and the user should, therefore, make his own phase boundary calculation.

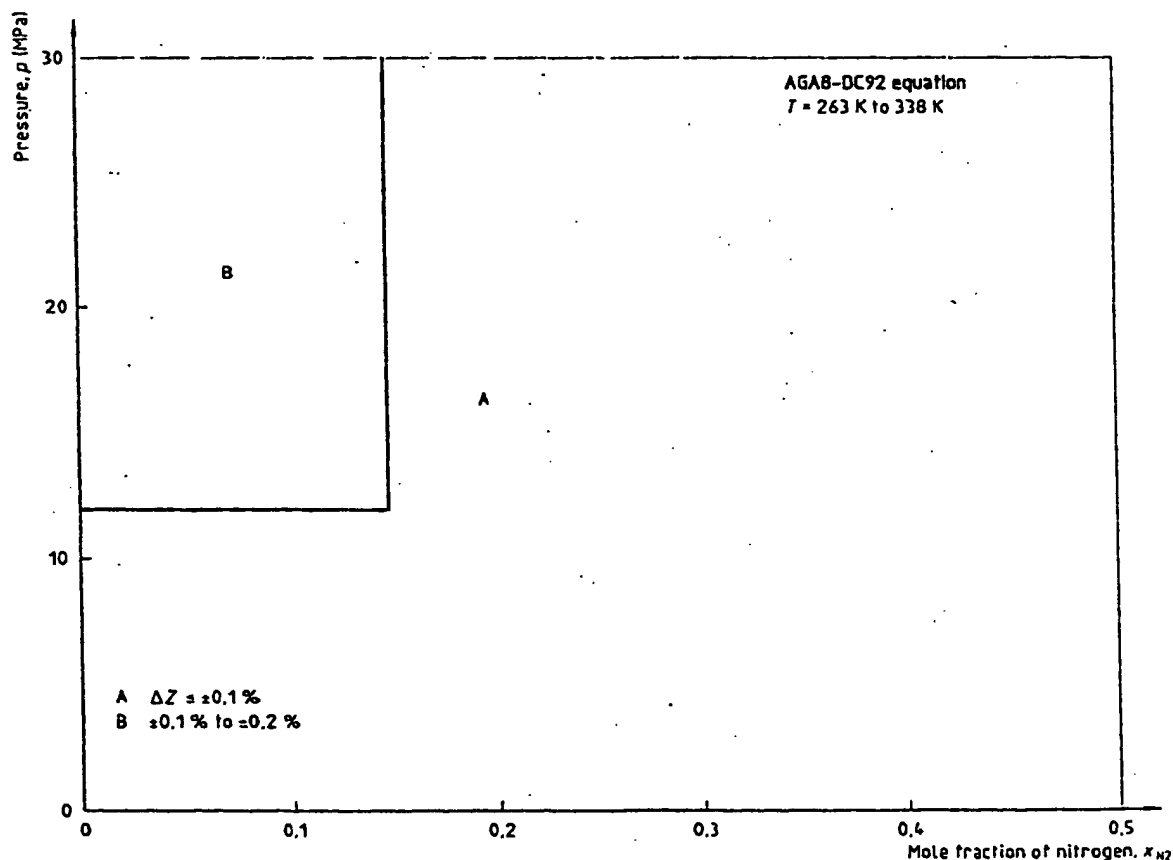


Figure E.1 — Estimated uncertainty limits for the calculation of compression factors of natural gases with a high nitrogen content

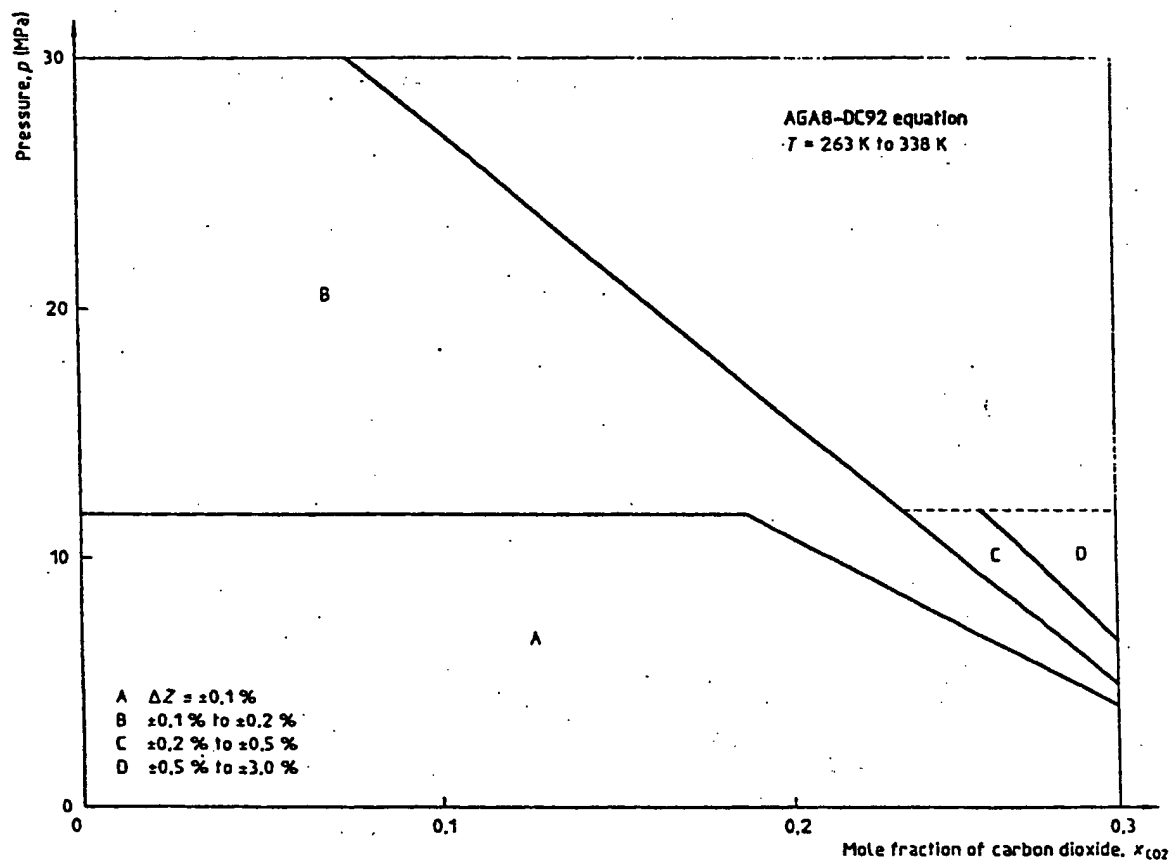


Figure E.2 — Estimated uncertainty limits for the calculation of compression factors of natural gases with a high carbon dioxide content

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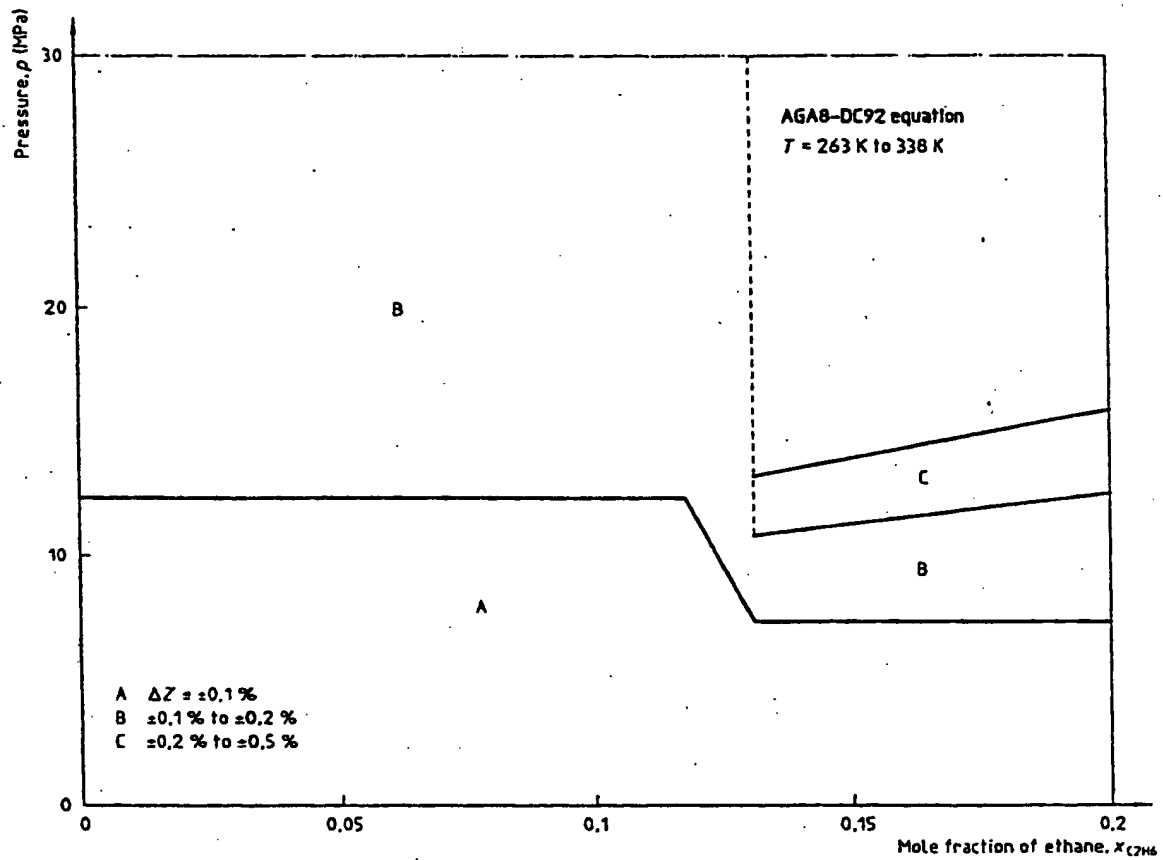


Figure E.3 — Estimated uncertainty limits for the calculation of compression factors of natural gases with a high ethane content

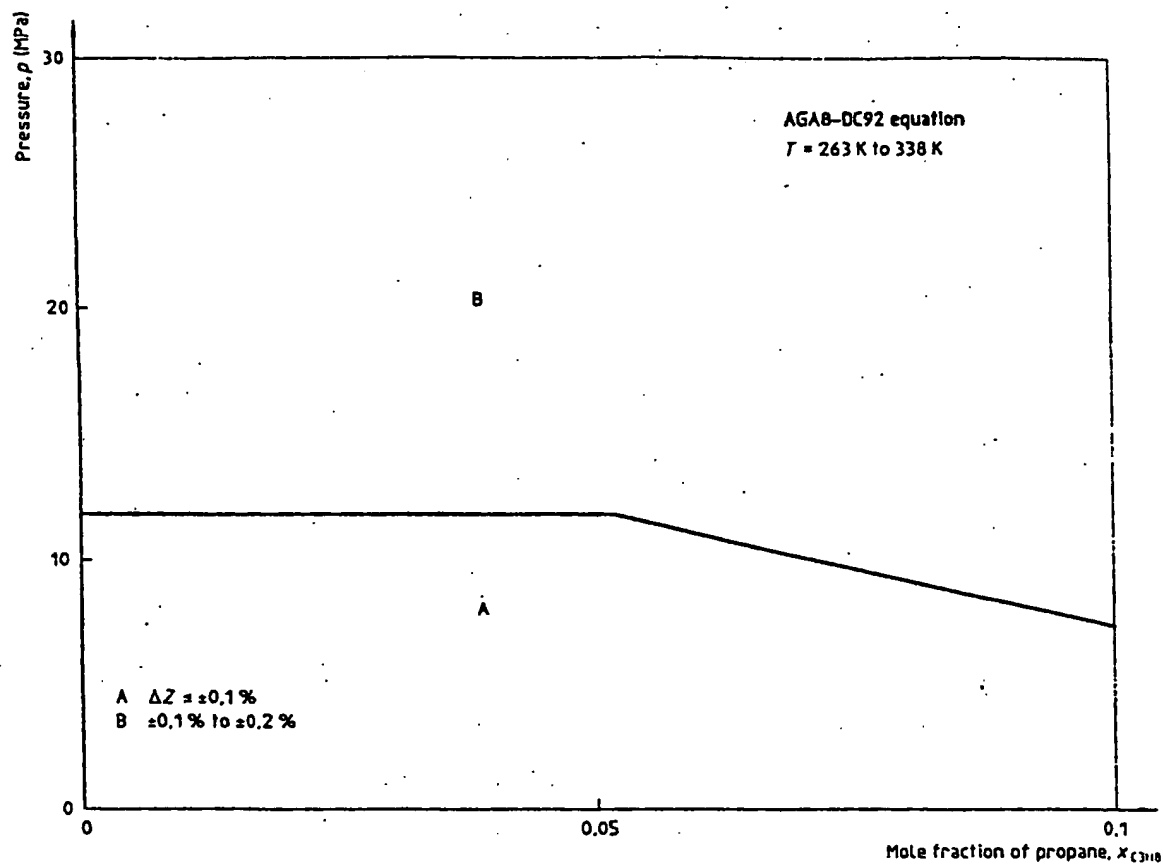


Figure E.4 — Estimated uncertainty limits for the calculation of compression factors of natural gases with a high propane content

The overall results at pressures up to 10 MPa and temperatures within the range 263 K to 338 K can be summarized as follows. Only gases having mole fractions within the limits given below will have uncertainties within $\pm 0,1 \%$, $\pm 0,2 \%$ and $\pm 0,5 \%$, respectively, within the given pressure and temperature domain.

| Component | Mole fraction for an uncertainty within | | |
|----------------|---|--------------|--------------|
| | $\pm 0,1 \%$ | $\pm 0,2 \%$ | $\pm 0,5 \%$ |
| Nitrogen | $\leq 0,50$ | — | — |
| Carbon dioxide | $\leq 0,23$ | $\leq 0,26$ | $\leq 0,28$ |
| Ethane | $\leq 0,13$ | $\leq 0,20$ | — |
| Propane | $\leq 0,06$ | $\leq 0,10$ | — |

Annex F (informative)

Subroutines in Fortran for the AGA8-92DC method

update: 17.05.94 E.W. Lemmon/S.W. Beyerlein/J.L. Savidge
update: 4.09.95 M. Jaeschke J. Sikora

=====

AGA8-DC92 COMPRESSION FACTOR EQUATION

=====

SUBROUTINE DCAGA

This program was written to accompany ISO 12213.

"DCAGA" Calculates the compression factor of natural gases using
a detailed gas analysis.

For information contact: DR. Jeffrey L. Savidge
gas research institute
8600 W. Bryn Mawr Ave.
Chicago, IL 60631
(312) 399-8100, FAX (312) 399-8125

This program calculates compression factors and molar densities for
natural gases from the input of gas composition in accordance with the
AGA8-DC92 compression equation developed by the Gas
Research Institute, Chicago, Illinois. (K.E. Starling and J.L.
Savidge, Compressibility Factors of Natural Gas and Other Related
Hydrocarbon Gases, American Gas Association, AGA Transmission
Measurement Committee Report No. 8, American Petroleum Institute MPMS
Chapter 14.2, Second Edition, November 1992, Catalog No. XQ9212).

The coefficients used in this program are the same as the values found
in AGA Report No. 8, November 1992.
Values for the gas constant and molar masses conform with ISO 6976
(1995) and GPA 2172 (1988).

Ranges of application for compression factor calculation
with the AGA8 - DC92 equation:

p-T-ranges
absolute pressure 0 to 65 MPa
temperature 225 to 350 K

Ranges for percentage molar composition:

A: pipeline quality natural gas
B: wider ranges of application

| | A | B |
|-----------------|-----------|-----------|
| methane | 70 to 100 | 50 to 100 |
| nitrogen | 0 to 20 | 0 to 50 |
| carbon dioxide | 0 to 20 | 0 to 30 |
| ethane | 0 to 10 | 0 to 20 |
| propane | 0 to 3.5 | 0 to 5 |
| butanes | 0 to 1.5 | 0 to 1.5 |
| pentanes | 0 to 0.5 | 0 to 0.5 |
| hexanes | 0 to 0.1 | 0 to 0.1 |
| heptanes | 0 to 0.05 | 0 to 0.05 |
| octanes plus | 0 to 0.05 | 0 to 0.05 |
| hydrogen | 0 to 10 | 0 to 10 |
| carbon monoxide | 0 to 3 | 0 to 3 |
| helium | 0 to 0.5 | 0 to 0.5 |

C water 0 to 0.015 0 to 0.015
 C
 C The expected uncertainty of the calculated results are for
 C pipeline quality natural gases:
 C +/- 0,1% within p-T range 0 to 12 MPa, 263 to 350 K
 C +/- 0,6% within p-T range 0 to 60 MPa, 225 to 350 K
 C The expected uncertainty in the wider range of application
 C (composition) is often even for pressures up to 12 MPa larger.
 C For more details see ISO 12213 part 2.
 C

SUBROUTINE DCAGA (XJ)

INTEGER B(58),C(58),K(58),G(58)
 INTEGER Q(58),F(58),S(58),W(58)
 REAL*8 A(58),U(58)
 COMMON /CONSTANTS/ A,B,C,K,U,G,Q,F,S,W

REAL*8 MW(21),EI(21),KI(21),GI(21),QI(21),FI(21),SI(21),WI(21)
 REAL*8 EIJ(21,21),UIJ(21,21),KIJ(21,21),GIJ(21,21)
 COMMON /PARAMETERS/ MW,EI,KI,GI,QI,FI,SI,WI,EIJ,UIJ,KIJ,GIJ

REAL*8 K1, CNS(58), BI(18)
 COMMON /COEF/ K1, CNS, BI

REAL*8 MWX, RGAS, TCM, DCM
 COMMON /MW/ MWX, RGAS, TCM, DCM

INTEGER I, J, N
 REAL*8 SUM, XI(21), XJ(21)
 REAL*8 U1, G1, Q1, F1, E1
 REAL*8 XIJ, EIJO, GIJO, BN

XI(1) = XJ(1)
 XI(4) = XJ(2)
 XI(5) = XJ(3)
 XI(11) = XJ(4)
 XI(12) = XJ(5)
 XI(13) = XJ(6)
 XI(14) = XJ(7)
 XI(15) = XJ(8)
 XI(16) = XJ(9)
 XI(17) = XJ(10)
 XI(18) = XJ(11)
 XI(19) = XJ(12)
 XI(3) = XJ(13)
 XI(2) = XJ(14)
 XI(7) = XJ(15)
 XI(20) = XJ(16)
 XI(6) = XJ(17)
 XI(10) = XJ(18)
 XI(21) = XJ(19)
 XI(8) = XJ(20)
 XI(9) = XJ(21)

C.....Normalize mole fractions

SUM = 0
 MWX = 0
 DO 10 I=1, 21
 10 SUM = SUM + XI(I)
 DO 20 I=1, 21
 20 XI(I) = XI(I)/SUM

C.....Calculate molecular weight

RGAS = 8.31451D-3
 MWX = 0
 DO 30 I=1, 21
 30 MWX = MWX + XI(I)*MW(I)
 DO 40 N=1, 18
 40 BI(N) = 0


```

K1 = 0
U1 = 0
G1 = 0
Q1 = 0
F1 = 0
E1 = 0

DO 50 I=1, 21
  K1 = K1 + XI(I)*KI(I)**2.5D0
  U1 = U1 + XI(I)*EI(I)**2.5D0
  G1 = G1 + XI(I)*GI(I)
  Q1 = Q1 + XI(I)*QI(I)
  F1 = F1 + XI(I)*XI(I)*FI(I)
  E1 = E1 + XI(I)*EI(I)
50 CONTINUE
  TCM = 1.261*E1
  DCM = K1**(-1.2D0)
  K1 = K1*K1
  U1 = U1*U1

  DO 60 I=1, 8
    DO 60 J=I+1, 19
      XIJ = XI(I)*XI(J)
      IF (XIJ.NE.0) THEN
        K1 = K1+2.D0*XIJ*(KIJ(I,J)**5.D0-1.D0)*(KI(I)*KI(J))**2.5D0
        U1 = U1+2.D0*XIJ*(UIJ(I,J)**5.D0-1.D0)*(EI(I)*EI(J))**2.5D0
        G1 = G1+XIJ*(GIJ(I,J) - 1.D0)*(GI(I) + GI(J))
      ENDIF
60 CONTINUE

  DO 80 I=1, 21
    DO 80 J=I, 21
      XIJ = XI(I)*XI(J)
      IF (XIJ.NE.0) THEN
        IF (I.NE.J) XIJ = 2.D0*XIJ
        EIJO = EIJ(I,J)*DSQRT(EI(I)*EI(J))
        GIJO = GIJ(I,J)*(GI(I) + GI(J))/2.D0
        DO 70 N=1, 18
          BN = (GIJO + 1.D0 - G(N))**G(N)
          &      * (QI(I)*QI(J) + 1.D0 - Q(N))**Q(N)
          &      * (DSQRT(FI(I)*FI(J)) + 1.D0 - F(N))**F(N)
          &      * (SI(I)*SI(J) + 1.D0 - S(N))**S(N)
          &      * (WI(I)*WI(J) + 1.D0 - W(N))**W(N)
          BI(N) = BI(N)+A(N)*XIJ*EIJO**U(N)*(KI(I)*KI(J))**1.5D0*BN
70 CONTINUE
        ENDIF
80 CONTINUE

    K1 = K1**0.2D0
    U1 = U1**0.2D0
    DO 90 N=13, 58
90 CNS(N) = (G1 + 1.D0 - G(N))**G(N)
    &      * (Q1**2 + 1.D0 - Q(N))**Q(N)
    &      * (F1 + 1.D0 - F(N))**F(N)
    &      * A(N)*U1**U(N)
    END
C=====
SUBROUTINE PZOFDT(D, T, P, Z, BMIX)

INTEGER B(58),C(58),K(58),G(58)
INTEGER Q(58),F(58),S(58),W(58)
REAL*8 A(58),U(58)
COMMON /CONSTANTS/ A,B,C,K,U,G,Q,F,S,W

REAL*8 K1, CNS(58), BI(18)
COMMON /COEF/ K1, CNS, BI

REAL*8 MWX, RGAS, TCM, DCM
COMMON /MW/ MWX, RGAS, TCM, DCM

```

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```

      INTEGER N
      REAL*8 D, T, P, Z, BMIX, DR

      DR = D*K1**3
      BMIX = 0
      DO 10 N=1, 18
10    BMIX = BMIX + BI(N)/T**U(N)

      Z = 1.D0 + BMIX*D
      DO 20 N=13, 18
20    Z = Z - DR*CNS(N)/T**U(N)

      DO 30 N=13, 58
30    Z = Z + CNS(N)/T**U(N)*(B(N) - C(N)*K(N)*DR**K(N))*DR**B(N)
      &    *DEXP(-C(N)*DR**K(N))
      P = D*RGAS*T*Z
      END
C=====
      SUBROUTINE DZOFPT(P, T, D, Z, BMIX)

      REAL*8 P, T, D, Z, BMIX
      REAL*8 X1, X2, X3, F, F1, F2, F3, TOL
      INTEGER I

      TOL = 0.5D-9
      X1 = 0.000001D0
      X2 = 40.D0
      D = 0

      CALL PZOFDT(X1, T, F1, Z, BMIX)
      CALL PZOFDT(X2, T, F2, Z, BMIX)
      F1 = F1 - P
      F2 = F2 - P
      IF (F1*F2.GE.0) RETURN
C-----
C  BEGIN ITERATING
C-----
      DO 60 I = 1, 50
C    ...Use False Position to get point 3.
      X3 = X1 - F1*(X2 - X1)/(F2 - F1)
      CALL PZOFDT(X3, T, F3, Z, BMIX)
      F3 = F3 - P

C    ...Use points 1, 2, and 3 to estimate the root using Chamber's
C    ...method (quadratic solution).
      D = X1*F2*F3/((F1 - F2)*(F1 - F3))
      &    + X2*F1*F3/((F2 - F1)*(F2 - F3))
      &    + X3*F1*F2/((F3 - F1)*(F3 - F2))
      IF ((D - X1)*(D - X2).GE.0) D = (X1 + X2)/2.D0
      CALL PZOFDT(D, T, F, Z, BMIX)
      F = F - P
      IF (DABS(F).LE.TOL) RETURN

C    ...Discard quadratic solution if false position root is closer.
      IF (DABS(F3).LT.DABS(F) .AND. F*F3.GT.0) THEN
        IF (F3*F1.GT.0) THEN
          X1 = X3
          F1 = F3
        ELSE
          X2 = X3
          F2 = F3
        ENDIF
      ELSE
        ...Swap in new value from quadratic solution
        IF (F*F3.LT.0) THEN
          X1 = D
          F1 = F
          X2 = X3

```

```

F2 = F3
ELSEIF (F3*F1.GT.0) THEN
  X1 = D
  F1 = F
ELSE
  X2 = D
  F2 = F
ENDIF
ENDIF
CONTINUE
D = 0
END
=====
BLOCK DATA
INTEGER B(58),C(58),K(58),G(58)
INTEGER Q(58),F(58),S(58),W(58)
REAL*8 A(58),U(58)
COMMON /CONSTANTS/ A,B,C,K,U,G,Q,F,S,W

REAL*8 MW(21),EI(21),KI(21),GI(21),QI(21),FI(21),SI(21),WI(21)
REAL*8 EIJ(21,21),UIJ(21,21),KIJ(21,21),GIJ(21,21)
COMMON /PARAMETERS/ MW,EI,KI,GI,QI,FI,SI,WI,EIJ,UIJ,KIJ,GIJ

REAL*8 XN(21), XH(21)
COMMON /GRENZDATA/ XN,XH

C.....Equation of state parameters
DATA A/
& 0.153832600D0, 1.341953000D0, -2.998583000D0, -0.048312280D0,
& 0.375796500D0, -1.589575000D0, -0.053588470D0, 0.886594630D0,
& -0.710237040D0, -1.471722000D0, 1.321850350D0, -0.786659250D0,
& 0.2291290D-08, 0.157672400D0, -0.436386400D0, -0.044081590D0,
& -0.003433888D0, 0.032059050D0, 0.024873550D0, 0.073322790D0,
& -0.001600573D0, 0.642470600D0, -0.416260100D0, -0.066899570D0,
& 0.279179500D0, -0.696605100D0, -0.002865089D0, -0.008098836D0,
& 3.150547000D0, 0.007224479D0, -0.705752900D0, 0.534979200D0,
& -0.079314910D0, -1.418465000D0, -0.5999050D-16, 0.105840200D0,
& 0.034317290D0, -0.007022847D0, 0.024955870D0, 0.042968180D0,
& 0.746545300D0, -0.291961300D0, 7.294616000D0, -9.936757000D0,
& -0.005399808D0, -0.243256700D0, 0.049870160D0, 0.003733797D0,
& 1.874951000D0, 0.002168144D0, -0.658716400D0, 0.000205518D0,
& 0.009776195D0, -0.020487080D0, 0.015573220D0, 0.006862415D0,
& -0.001226752D0, 0.002850908D0/
DATA B/1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,2,2,2,2,2,2,2,2,3,3,3,3,
& 3,3,3,3,3,3,3,3,4,4,4,4,4,4,4,5,5,5,5,5,6,6,7,7,8,8,8,9,9/
DATA C/0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,1,1,1,1,1,0,0,1,1,1,1,1,1,1,0,1,
& 1,1,1,1,1,1,1,1,0,0,1,1,1,1,1,1,0,0,1,1,1,1,0,1,0,1,1,1,1,1,1/
DATA K/0,0,0,0,0,0,0,0,0,0,0,0,0,0,3,2,2,2,4,4,0,0,2,2,2,4,4,4,4,0,1,
& 1,2,2,3,3,4,4,4,0,0,2,2,2,4,4,0,2,2,4,4,0,2,0,2,1,2,2,2,2/
DATA G/0,0,0,0,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,0,1,
& 0,0,1,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,1,0,1,0/
DATA Q/0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,0,1,0,
& 0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1/
DATA F/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,
& 1,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA S/0,0,0,0,0,0,0,0,0,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,
& 0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA W/0,0,0,0,0,0,0,0,0,0,0,0,0,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,
& 0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA U/0,0,5D0,1,3,5D0,-0,5D0,4,5D0,0,5D0,7,5D0,9,5D0,6,12,12,5D0
& -6,2,3,2,2,11,-0,5D0,0,5D0,0,4,6,21,23,22,-1,-0,5D0,7,-1,6,
& 4,1,9,-13,21,8,-0,5D0,0,2,7,9,22,23,1,9,3,8,23,1,5D0,5,
& -0,5D0,4,7,3,0,1,0/

C.....Characterization Parameters
DATA MW/16.0430D0, 28.0135D0, 44.0100D0, 30.0700D0, 44.0970D0,
& 18.0153D0, 34.0820D0, 2.0159D0, 28.0100D0, 31.9988D0,
& 58.1230D0, 58.1230D0, 72.1500D0, 72.1500D0, 86.1770D0,
& 100.2040D0,114.2310D0,128.2580D0,142.2850D0, 4.0026D0,
& 39.9480D0/

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DATA EI/151.318300D0, 99.737780D0, 241.960600D0, 244.166700D0,
& 298.118300D0, 514.015600D0, 296.355000D0, 26.957940D0,
& 105.534800D0, 122.766700D0, 324.068900D0, 337.638900D0,
& 365.599900D0, 370.682300D0, 402.636293D0, 427.722630D0,
& 450.325022D0, 470.840891D0, 489.558373D0, 2.610111D0,
& 119.629900D0/
DATA KI/0.4619255D0, 0.4479153D0, 0.4557489D0, 0.5279209D0,
& 0.5837490D0, 0.3825868D0, 0.4618263D0, 0.3514916D0,
& 0.4533894D0, 0.4186954D0, 0.6406937D0, 0.6341423D0,
& 0.6738577D0, 0.6798307D0, 0.7175118D0, 0.7525189D0,
& 0.7849550D0, 0.8152731D0, 0.8437826D0, 0.3589888D0,
& 0.4216551D0/
DATA GI/0, 0.027815D0, 0.189065D0, 0.079300D0, 0.141239D0,
& 0.332500D0, 0.088500D0, 0.034369D0, 0.038953D0, 0.021000D0,
& 0.256692D0, 0.281835D0, 0.332267D0, 0.366911D0, 0.289731D0,
& 0.337542D0, 0.383381D0, 0.427354D0, 0.469659D0, 0, 0/
DATA QI/2*0, 0.69D0, 2*0, 1.06775D0, 0.633276D0, 14*0/
DATA FI/7*0, 1, 13*0/
DATA SI/5*0, 1.5822D0, 0.390D0, 14*0/
DATA WI/5*0, 1, 15*0/

```

C.....Binary interaction parameters

```

DATA EIJ/441*1/
DATA UIJ/441*1/
DATA KIJ/441*1/
DATA GIJ/441*1/

```

```

DATA (EIJ(1,J),J=2,19)/
& 0.971640D0, 0.960644D0, 1, 0.994635D0, 0.708218D0,
& 0.931484D0, 1.170520D0, 0.990126D0, 1, 1.019530D0,
& 0.989844D0, 1.002350D0, 0.999268D0, 1.107274D0, 0.880880D0,
& 0.880973D0, 0.881067D0, 0.881161D0/
DATA (EIJ(2,J),J=3,14)/
& 1.022740D0, 0.970120D0, 0.945939D0, 0.746954D0, 0.902271D0,
& 1.086320D0, 1.005710D0, 1.021000D0, 0.946914D0, 0.973384D0,
& 0.959340D0, 0.945520D0/
DATA (EIJ(3,J),J=4,19)/
& 0.925053D0, 0.960237D0, 0.849408D0, 0.955052D0, 1.281790D0,
& 1.5D0, 1, 0.906849D0, 0.897362D0, 0.726255D0,
& 0.859764D0, 0.855134D0, 0.831229D0, 0.808310D0, 0.786323D0,
& 0.765171D0/
DATA (EIJ(4,J),J=5,14)/1.022560D0, 0.693168D0, 0.946871D0,
& 1.164460D0, 3*1, 1.013060D0, 1, 1.005320D0/
DATA (EIJ(5,J),J=8,12)/1.034787D0, 3*1, 1.0049D0/
DATA (EIJ(7,J),J=15,19)/1.008692D0, 1.010126D0, 1.011501D0,
& 1.012821D0, 1.014089D0/
DATA (EIJ(8,J),J=9,12)/1.1D0, 1, 1.3D0, 1.3D0/

DATA (UIJ(1,J),J=2,19)/
& 0.886106D0, 0.963827D0, 1, 0.990877D0, 1, 0.736833D0,
& 1.156390D0, 3*1, 0.992291D0, 1, 1.003670D0, 1.302576D0,
& 1.191904D0, 1.205769D0, 1.219634D0, 1.233498D0/
DATA (UIJ(2,J),J=3,12)/0.835058D0, 0.816431D0, 0.915502D0, 1,
& 0.993476D0, 0.408838D0, 3*1, 0.993556D0/
DATA (UIJ(3,J),J=4,19)/0.969870D0, 2*1, 1.045290D0, 1, 0.9D0,
& 5*1, 1.066638D0, 1.077634D0, 1.088178D0, 1.098291D0,
& 1.108021D0/
DATA (UIJ(4,J),J=5,14)/
& 1.065173D0, 1, 0.971926D0, 1.616660D0, 2*1, 4*1.25D0/
DATA (UIJ(7,J),J=7,19)/8*1, 1.028973D0, 1.033754D0,
& 1.038338D0, 1.042735D0, 1.046966D0/

DATA (KIJ(1,J),J=2,19)/
& 1.003630D0, 0.995933D0, 1, 1.007619D0, 1, 1.000080D0,
& 1.023260D0, 3*1, 0.997596D0, 1, 1.002529D0, 0.982962D0,
& 0.983565D0, 0.982707D0, 0.981849D0, 0.980991D0/
DATA (KIJ(2,J),J=3,8)/
& 0.982361D0, 1.007960D0, 1, 1, 0.942596D0, 1.032270D0/
DATA (KIJ(3,J),J=4,19)/1.008510D0, 2*1, 1.00779D0, 7*1.0D0,
& 0.910183D0, 0.895362D0, 0.881152D0, 0.867520D0, 0.854406D0/

```

```
DATA (KIJ(4,J),J=5,8)/0.986893D0, 1, 0.999969D0, 1.020340D0/
DATA (KIJ(7,J),J=7,21)/8*1, 0.968130D0, 0.962870D0,
& 0.957828D0, 0.952441D0, 0.948338D0, 2*1/
```

```
DATA GIJ(1,3) /0.807653D0/
DATA GIJ(1,8) /1.957310D0/
DATA GIJ(2,3) /0.982746D0/
DATA GIJ(3,4) /0.370296D0/
DATA GIJ(3,6) /1.673090D0/
```

C

```
DATA XN/
& 50.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 ,
& 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 ,
& 0.0 , 0.0 , 0.0 , 0.0 , 0.0 /
```

C

```
DATA XH/
& 100.0 , 20.0 , 5.0 , 1.5 , 1.5 , 0.5 , 0.5 , 0.1 ,
& 0.05 , 0.05 , 0.05 , 0.05 , 30.0 , 50.0 , 0.02 , 0.5 ,
& 0.015, 0.02 , 0.02 , 10.0 , 3.0/
END
```

Annex G (informative)

Bibliography

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**INTERNATIONAL
STANDARD**

**ISO
12213-3**

First edition
1997-12-01

**Natural gas — Calculation of compression
factor —**

**Part 3:
Calculation using physical properties**

Gaz naturel — Calcul du facteur de compression —

Partie 3: Calcul au moyen des caractéristiques physiques



Reference number
ISO 12213-3:1997(E)

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Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

Draft International Standards adopted by the technical committees are circulated to the member bodies for voting. Publication as an International Standard requires approval by at least 75 % of the member bodies casting a vote.

International Standard ISO 12213-3 was prepared by Technical Committee ISO/TC 193, *Natural gas*, Subcommittee SC 1, *Analysis of natural gas*.

ISO 12213 consists of the following parts, under the general title *Natural gas* — *Calculation of compression factor*.

- *Part 1: Introduction and guidelines*
- *Part 2: Calculation using molar-composition analysis*
- *Part 3: Calculation using physical properties*

Annexes A to D form an integral part of this part of ISO 12213. Annexes E to G are for information only.

Natural gas — Calculation of compression factor —

Part 3: Calculation using physical properties

1 Scope

This International Standard specifies methods for the calculation of compression factors of natural gases, natural gases containing a synthetic admixture and similar mixtures at conditions under which the mixture can exist only as a gas.

This part of ISO 12213 specifies a method for the calculation of compression factors when the superior calorific value, relative density and carbon dioxide content are known, together with the relevant pressures and temperatures. If hydrogen is present, as is often the case for gases with a synthetic admixture, the hydrogen content also needs to be known.

NOTE — In principle, it is possible to calculate the compression factor when any three of the parameters superior calorific value, relative density, carbon dioxide content (the usual three) and nitrogen content are known, but subsets including nitrogen content are not recommended.

The method is primarily applicable to pipeline quality gases within the ranges of pressure p and temperature T at which transmission and distribution operations normally take place, with an uncertainty of about $\pm 0,1\%$. For wider-ranging applications the uncertainty of the results increases (see annex E).

More detail concerning the scope and field of application of the method is given in part 1 of this International Standard.

2 Normative references

The following standards contain provisions which, through reference in this text, constitute provisions of this part of ISO 12213. At the time of publication, the editions indicated were valid. All standards are subject to revision, and parties to agreements based on this part of ISO 12213 are encouraged to investigate the possibility of applying the most recent editions of the standards indicated below. Members of IEC and ISO maintain registers of currently valid International Standards.

ISO 31-3:1992, *Quantities and units — Part 3: Mechanics*.

ISO 31-4:1992, *Quantities and units — Part 4: Heat*.

ISO 6976:1995, *Natural gas — Calculation of calorific values, density, relative density and Wobbe index from composition*.

ISO 12213-1:1997, *Natural gas — Calculation of compression factor — Part 1: Introduction and guidelines*.

3 Definitions

All definitions relevant to the use of this part of ISO 12213 are given in part 1.

4 Method of calculation

4.1 Principle

The method recommended uses equations which are based on the concept that pipeline quality natural gas may be uniquely characterized for calculation of its volumetric properties by an appropriate and distinctive set of measurable physical properties. These characteristics, together with the pressure and temperature, are used as input data for the method.

The method uses the following physical properties: superior calorific value, relative density and carbon dioxide content. The method is particularly useful in the common situation where a complete molar composition is not available, but may also be preferred for its relative simplicity. For gases with a synthetic admixture, the hydrogen content needs to be known.

4.2 The SGERG-88 equation

The calculation method using physical properties is based on the standard GERG 88 (SGERG-88) virial equation for natural gases [1], [2], [3]. The standard GERG 88 virial equation is derived from the master GERG 88 (MGERG-88) virial equation, which is a method of calculation based on a molar-composition analysis [4].

The SGERG-88 virial equation from which the compression factor Z is calculated may be written as

$$Z = 1 + B\rho_m + C\rho_m^2 \quad \dots (1)$$

where

B and C are functions of the input data comprising the superior calorific value H_S , the relative density d , the contents of both inert and combustible non-hydrocarbon components of the gas mixture (CO_2 and H_2) and the temperature T ;

ρ_m is the molar density given by

$$\rho_m = p/(ZRT) \quad \dots (2)$$

where

$$Z = f_1(p, T, H_S, d, x_{\text{CO}_2}, x_{\text{H}_2}) \quad \dots (3)$$

However, the SGERG-88 method treats the natural-gas mixture internally as a five-component mixture consisting of an equivalent hydrocarbon gas (with the same thermodynamic properties as the sum of the hydrocarbons present), nitrogen, carbon dioxide, hydrogen and carbon monoxide. To characterize the thermodynamic properties of the hydrocarbon gas adequately, the hydrocarbon heating value H_{CH} is also needed. Therefore, the calculation of Z uses

$$Z = f_2(p, T, H_{\text{CH}}, x_{\text{CH}}, x_{\text{N}_2}, x_{\text{CO}_2}, x_{\text{H}_2}, x_{\text{CO}}) \quad \dots (4)$$

In order to be able to model coke oven gas mixtures, the mole fraction of carbon monoxide is taken to have a fixed relation to the hydrogen content. If hydrogen is not present ($x_{\text{H}_2} < 0,001$), then set $x_{\text{H}_2} = 0$. The natural-gas mixture is then treated in the calculation method as a three-component mixture (see annex B).

The calculation is performed in three steps.

First, the five-component composition from which both the known superior calorific value and the known relative density can be calculated satisfactorily may be found from the input data by an iterative procedure described in detail in annex B.

Secondly, once this composition is known, B and C may be found using relationships also given in annex B.

In the third step, equations (1) and (2) are solved simultaneously for ρ_m and Z by a suitable numerical method.

A flow diagram of the procedure for calculating Z from the input data is shown in figure B.1.

4.3 Input variables

4.3.1 Preferred input data set

The input variables required for use with the SGERG-88 equation are the absolute pressure, temperature and superior calorific value (volumetric basis), the relative density, the carbon dioxide content and the hydrogen content. Thus the physical properties used the input data set (set A) are

$$H_S, d, x_{CO_2} \text{ and } x_{H_2}$$

Relative density is referred to normal conditions (101,325 kPa and 0 °C) and superior calorific value is referred to normal conditions (101,325 kPa and 0 °C) and a combustion temperature of 25 °C.

4.3.2 Alternative input data sets

Three alternatives to the preferred input data set (see 4.3.1) may be used with the standard GERG virial equation:

$$x_{N_2}, H_S, d \text{ and } x_{H_2} \text{ (set B)}$$

$$x_{N_2}, x_{CO_2}, d \text{ and } x_{H_2} \text{ (set C)}$$

$$x_{N_2}, x_{CO_2}, H_S \text{ and } x_{H_2} \text{ (set D)}$$

The alternative input data sets are considered fully in GERG Technical Monograph TM5 [3]. Use of the alternative input data sets gives results which may differ at the fourth decimal place. This part of ISO 12213 recommends the use of input data set A.

4.4 Ranges of application

4.4.1 Pipeline quality gas

The ranges of application for pipeline quality gas are as defined below:

| | | | |
|---------------------------------|-----------------------|-----------------|------------------------------|
| absolute pressure | 0 MPa | $\leq p$ | ≤ 12 MPa |
| temperature | 263 K | $\leq T$ | ≤ 338 K |
| mole fraction of carbon dioxide | 0 | $\leq x_{CO_2}$ | $\leq 0,20$ |
| mole fraction of hydrogen | 0 | $\leq x_{H_2}$ | $\leq 0,10$ |
| superior calorific value | 30 MJ·m ⁻³ | $\leq H_S$ | ≤ 45 MJ·m ⁻³ |
| relative density | 0,55 0,71 | $\leq d$ | $\leq 0,80$ 1,03 |

The mole fractions of other natural-gas components are not required as input. These mole fractions shall, however, lie within the following ranges:

| | |
|----------|-------------------------------------|
| methane | 0,7 $\leq x_{CH_4}$ $\leq 1,0$ |
| nitrogen | 0 $\leq x_{N_2}$ $\leq 0,20$ |
| ethane | 0 $\leq x_{C_2H_6}$ $\leq 0,10$ |
| propane | 0 $\leq x_{C_3H_8}$ $\leq 0,035$ |
| butanes | 0 $\leq x_{C_4H_{10}}$ $\leq 0,015$ |

| | |
|----------------------------------|-----------------------------------|
| pentanes | $0 \leq x_{C_5H_{12}} \leq 0,005$ |
| hexanes | $0 \leq x_{C_6} \leq 0,001$ |
| heptanes | $0 \leq x_{C_7} \leq 0,000\ 5$ |
| octanes plus higher hydrocarbons | $0 \leq x_{C_{8+}} \leq 0,000\ 5$ |
| carbon monoxide | $0 \leq x_{CO} \leq 0,03$ |
| helium | $0 \leq x_{He} \leq 0,005$ |
| water | $0 \leq x_{H_2O} \leq 0,000\ 15$ |

The method applies only to mixtures in the single-phase gaseous state (above the dew point) at the conditions of temperature and pressure of interest. For pipeline quality, the method is applicable over wider ranges of temperature and pressure but with increased uncertainty (see figure 1). In the computer implementation, the lower temperature limit is set at 250 K.

4.4.2 Wider ranges of application

The ranges of application tested beyond the limits given in 4.4.1 are:

| | |
|---------------------------------|---|
| absolute pressure | $0\text{ MPa} \leq p \leq 12\text{ MPa}$ |
| temperature | $263\text{ K} \leq T \leq 338\text{ K}$ |
| mole fraction of carbon dioxide | $0 \leq x_{CO_2} \leq 0,30$ |
| mole fraction of hydrogen | $0 \leq x_{H_2} \leq 0,10$ |
| superior calorific value | $20\text{ MJ}\cdot\text{m}^{-3} \leq H_S \leq 48\text{ MJ}\cdot\text{m}^{-3}$ |
| relative density | $0,55 \leq d \leq 0,90$ 1,16 |

The allowable mole fractions of other major natural-gas components are extended to:

| | |
|----------|-------------------------------|
| methane | $0,5 \leq x_{CH_4} \leq 1,0$ |
| nitrogen | $0 \leq x_{N_2} \leq 0,50$ |
| ethane | $0 \leq x_{C_2H_6} \leq 0,20$ |
| propane | $0 \leq x_{C_3H_8} \leq 0,05$ |

The limits for other minor natural-gas components remain as given in 4.4.1 for pipeline quality gas.

The method is not applicable outside these ranges; the computer implementation described in annex B will not allow violation of the limits of composition quoted here.

4.5 Uncertainty

4.5.1 Uncertainty for pipeline quality gas

The uncertainty in the prediction of the compression factor ΔZ (for the temperature range 263 K to 338 K) is $\pm 0,1\%$ at pressures up to 10 MPa and $\pm 0,2\%$ between 10 MPa and 12 MPa for natural gases with $x_{N_2} \leq 0,20$, $x_{CO_2} \leq 0,09$, $x_{C_2H_6} \leq 0,10$ and $x_{H_2} \leq 0,10$, and for $30\text{ MJ}\cdot\text{m}^{-3} \leq H_S \leq 45\text{ MJ}\cdot\text{m}^{-3}$ and $0,55 \leq d \leq 0,80$, (see figure 1).

For gases with a CO_2 content exceeding 0,09, the uncertainty of $\pm 0,1\%$ is maintained for pressures up to 6 MPa and for temperatures between 263 K and 338 K. This uncertainty level is determined by comparison with the GERG databank on measurements of the compression factor for natural gases [5], [6] and with the Gas Research Institute data [9].

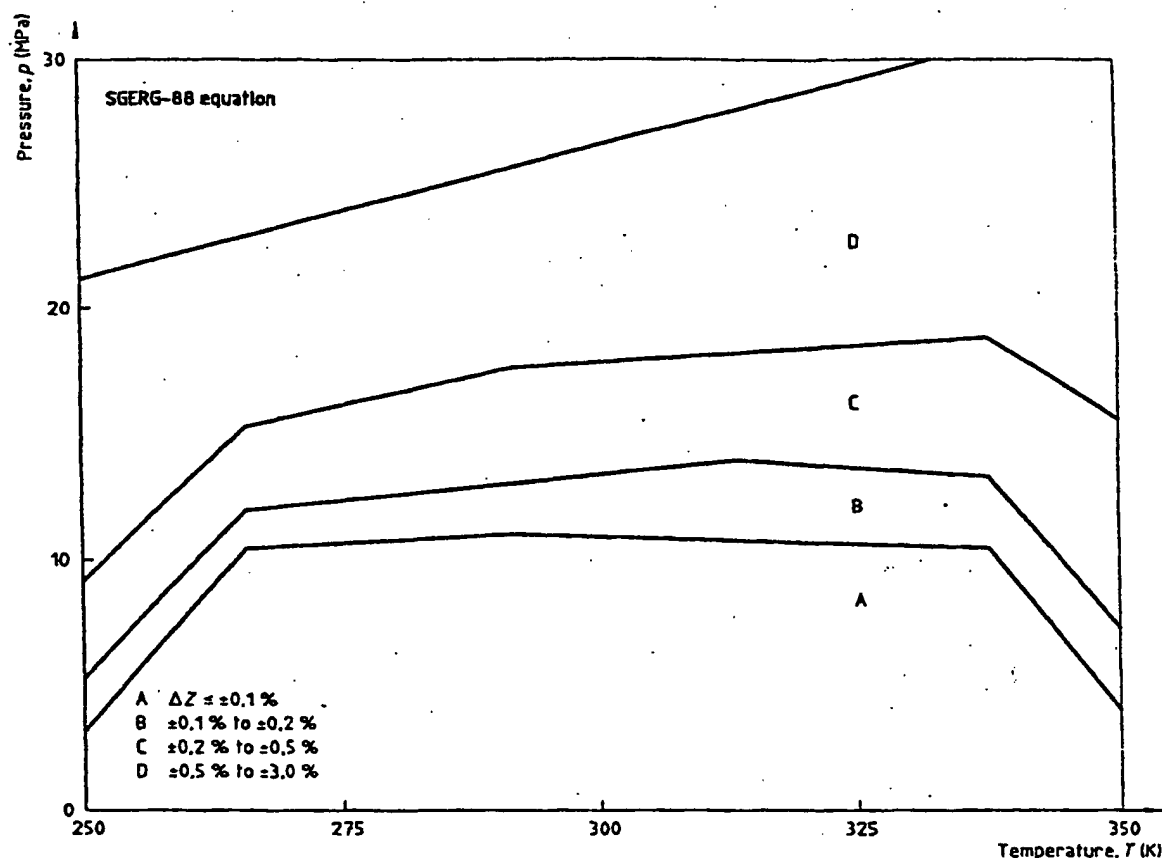


Figure 1 — Uncertainty limits for the calculation of compression factors (The uncertainty limits given are expected to be valid for natural gases and similar gases with $x_{N_2} \leq 0,20$; $x_{CO_2} \leq 0,09$; $x_{C_2H_6} \leq 0,10$ and $x_{H_2} \leq 0,10$, and for $30 \text{ MJ}\cdot\text{m}^{-3} \leq H_S \leq 45 \text{ MJ}\cdot\text{m}^{-3}$ and $0,55 \leq d \leq 0,80$)

4.5.2 Uncertainty for wider ranges of application

The estimated uncertainties involved in calculations of compression factors beyond the limits of quality given in 4.5.1 are discussed in annex E.

4.5.3 Impact of uncertainties of input variables

Listed in table 1 are typical values for the uncertainties of the relevant input variables. These values may be achieved under optimum operating conditions.

As a general guideline only, an error propagation analysis using the above uncertainties in the input variables produces an additional uncertainty of about $\pm 0,1 \%$ in the result at 6 MPa and within the temperature range 263 K to 338 K. Above 6 MPa, the additional uncertainties are greater and increase roughly in direct proportion to the pressure (see reference [3]).

4.5.4 Reporting of results

Results for the compression factor shall be reported to four places of decimals, together with the pressure and temperature values and the calculation method used (ISO 12213-3, SGERG 88 equation). For verification of calculation procedures, it is useful to carry extra digits.

Table 1 — Uncertainties of input variables

| Input variable | Absolute uncertainty |
|---------------------------------|-------------------------------|
| Absolute pressure | $\pm 0,02$ MPa |
| Temperature | $\pm 0,15$ K |
| Mole fraction of carbon dioxide | $\pm 0,002$ |
| Mole fraction of hydrogen | $\pm 0,005$ |
| Relative density | $\pm 0,001$ 3 |
| Superior calorific value | $\pm 0,06$ MJ·m ⁻³ |

5 Suppliers of computer programmes

It is planned to make software available which implements this International Standard. Users are invited to contact their ISO member body or ISO Central Secretariat to enquire about the availability of such software.

Annex A (normative)

Symbols and units

The symbols specified in this annex are those which are used in both the main text and in annex B. The units specified here are those which give consistency with the values of the coefficients given in annex B.

| Symbol | Meaning | Units |
|--------------|--|--|
| b_{H0} | Zero-order (constant) term in the molar heating value (H_{CH}) expansion of B_{11} [equation (B.20)] | $\text{m}^3 \cdot \text{kmol}^{-1}$ |
| b_{H1} | First-order (linear) term in the molar heating value (H_{CH}) expansion of B_{11} [equation (B.20)] | $\text{m}^3 \cdot \text{MJ}^{-1}$ |
| b_{H2} | Second-order (quadratic) term in the molar heating value (H_{CH}) expansion of B_{11} [equation (B.20)] | $\text{m}^3 \cdot \text{kmol}^{-1} \cdot \text{MJ}^{-2}$ |
| $b_{H0(0)}$ | Terms in the temperature expansion of b_{H0} [equation (B.21)] | $\text{m}^3 \cdot \text{kmol}^{-1}$ |
| $b_{H0(1)}$ | | $\text{m}^3 \cdot \text{kmol}^{-1} \cdot \text{K}^{-1}$ |
| $b_{H0(2)}$ | | $\text{m}^3 \cdot \text{kmol}^{-1} \cdot \text{K}^{-2}$ |
| $b_{H1(0)}$ | Terms in the temperature expansion of b_{H1} [equation (B.21)] | $\text{m}^3 \cdot \text{MJ}^{-1}$ |
| $b_{H1(1)}$ | | $\text{m}^3 \cdot \text{MJ}^{-1} \cdot \text{K}^{-1}$ |
| $b_{H1(2)}$ | | $\text{m}^3 \cdot \text{MJ}^{-1} \cdot \text{K}^{-2}$ |
| $b_{H2(0)}$ | Terms in the temperature expansion of b_{H2} [equation (B.21)] | $\text{m}^3 \cdot \text{kmol}^{-1} \cdot \text{MJ}^{-2}$ |
| $b_{H2(1)}$ | | $\text{m}^3 \cdot \text{kmol}^{-1} \cdot \text{MJ}^{-2} \cdot \text{K}^{-1}$ |
| $b_{H2(2)}$ | | $\text{m}^3 \cdot \text{kmol}^{-1} \cdot \text{MJ}^{-2} \cdot \text{K}^{-2}$ |
| $b_{ij(0)}$ | Terms in the temperature expansion of b_{ij} [equation (B.22)] | $\text{m}^3 \cdot \text{kmol}^{-1}$ |
| $b_{ij(1)}$ | | $\text{m}^3 \cdot \text{kmol}^{-1} \cdot \text{K}^{-1}$ |
| $b_{ij(2)}$ | | $\text{m}^3 \cdot \text{kmol}^{-1} \cdot \text{K}^{-2}$ |
| B | Second virial coefficient [equation (1)] | $\text{m}^3 \cdot \text{kmol}^{-1}$ |
| B_{ij} | Second virial coefficient for binary interaction between component i and component j [equation (B.22)] | $\text{m}^3 \cdot \text{kmol}^{-1}$ |
| c_{H0} | Zero-order (constant) term in the molar heating value (H_{CH}) expansion of C_{111} [equation (B.29)] | $\text{m}^6 \cdot \text{kmol}^{-2}$ |
| c_{H1} | First-order (linear) term in the molar heating value (H_{CH}) expansion of C_{111} [equation (B.29)] | $\text{m}^6 \cdot \text{kmol}^{-1} \cdot \text{MJ}^{-1}$ |
| c_{H2} | Second-order (quadratic) term in the molar heating value (H_{CH}) expansion of C_{111} [equation (B.29)] | $\text{m}^6 \cdot \text{MJ}^{-2}$ |
| $c_{H0(0)}$ | Terms in the temperature expansion of c_{H0} [equation (B.30)] | $\text{m}^6 \cdot \text{kmol}^{-2}$ |
| $c_{H0(1)}$ | | $\text{m}^6 \cdot \text{kmol}^{-2} \cdot \text{K}^{-1}$ |
| $c_{H0(2)}$ | | $\text{m}^6 \cdot \text{kmol}^{-2} \cdot \text{K}^{-2}$ |
| $c_{H1(0)}$ | Terms in the temperature expansion of c_{H1} [equation (B.30)] | $\text{m}^6 \cdot \text{kmol}^{-1} \cdot \text{MJ}^{-1}$ |
| $c_{H1(1)}$ | | $\text{m}^6 \cdot \text{kmol}^{-1} \cdot \text{MJ}^{-1} \cdot \text{K}^{-1}$ |
| $c_{H1(2)}$ | | $\text{m}^6 \cdot \text{kmol}^{-1} \cdot \text{MJ}^{-1} \cdot \text{K}^{-2}$ |
| $c_{H2(0)}$ | Terms in the temperature expansion of c_{H2} [equation (B.30)] | $\text{m}^6 \cdot \text{MJ}^{-2}$ |
| $c_{H2(1)}$ | | $\text{m}^6 \cdot \text{MJ}^{-2} \cdot \text{K}^{-1}$ |
| $c_{H2(2)}$ | | $\text{m}^6 \cdot \text{MJ}^{-2} \cdot \text{K}^{-2}$ |
| $c_{ijk(0)}$ | Terms in the temperature expansion of c_{ij} [equation (B.31)] | $\text{m}^6 \cdot \text{kmol}^{-2}$ |
| $c_{ijk(1)}$ | | $\text{m}^6 \cdot \text{kmol}^{-2} \cdot \text{K}^{-1}$ |
| $c_{ijk(2)}$ | | $\text{m}^6 \cdot \text{kmol}^{-2} \cdot \text{K}^{-2}$ |
| C | Third virial coefficient [equation (1)] | $\text{m}^6 \cdot \text{kmol}^{-2}$ |

| Symbol | Meaning | Units |
|-------------------|---|--|
| C_{ijk} | Third virial coefficient for ternary interaction between components i , j and k [equation (B.31)] | $\text{m}^6 \cdot \text{kmol}^{-2}$ |
| d | Relative density [$d(\text{air}) = 1$; equation (B.1)] | — |
| DH_{CH} | Change in the molar heating value H_{CH} during iteration [equations (B.10) and (B.11)] | $\text{MJ} \cdot \text{kmol}^{-1}$ |
| H_{S} | Superior calorific value [gas at normal conditions (0 °C, 1,013 25 bar), combustion temperature 25 °C] | $\text{MJ} \cdot \text{m}^{-3}$ |
| H | Molar heating value (combustion temperature 25 °C) | $\text{MJ} \cdot \text{kmol}^{-1}$ |
| M | Molar mass [equations (B.5) and (B.8)] | $\text{kg} \cdot \text{kmol}^{-1}$ |
| p | Absolute pressure | bar |
| R | (Universal) gas constant | $\text{m}^3 \cdot \text{bar} \cdot \text{kmol}^{-1} \cdot \text{K}^{-1}$ |
| T | Absolute temperature | K |
| t | Celsius temperature [= $T - 273,15$; equation (B.27)] | °C |
| V_{m} | Molar volume (= $1/\rho_{\text{m}}$) | $\text{m}^3 \cdot \text{kmol}^{-1}$ |
| x | Mole fraction of a component | — |
| y | Combination rule parameters for the binary unlike-interaction virial coefficients B_{12} and B_{13} (table B.1) and the ternary unlike-interaction virial coefficient C_{ijk} [equation (B.32)] | — |
| Z | Compression factor | — |
| ρ | Mass density [equations (B.8) and (B.42)] | $\text{kg} \cdot \text{m}^{-3}$ |
| ρ_{m} | Molar density (= V_{m}^{-1}) | $\text{kmol} \cdot \text{m}^{-3}$ |

Additional subscripts

| | |
|-----------------|--|
| n | Value at normal conditions ($T_n = 273,15 \text{ K}$, $p_n = 1,013 25 \text{ bar}$) |
| CH | For the equivalent hydrocarbon |
| CO | For carbon monoxide |
| CO ₂ | For carbon dioxide |
| H ₂ | For hydrogen |
| N ₂ | For nitrogen |

Additional qualifiers

| | |
|-----------|--|
| (air) | For dry air of standard composition [equation (B.1)] |
| (D) | For special value of ρ used in equation (B.11) |
| 1 | For the equivalent hydrocarbon [equations (B.12) and (B.15)] |
| 2 | For nitrogen [equations (B.12) and (B.16)] |
| 3 | For carbon dioxide [equations (B.12) and (B.17)] |
| 4 | For hydrogen [equations (B.12) and (B.18)] |
| 5 | For carbon monoxide [equations (B.12) and (B.19)] |
| (id) | Ideal gas state |
| (μ) | Iteration counter (B.2.1) |
| (ν) | Iteration counter (B.2.2) |
| (w) | Iteration counter (B.4) |

Annex B (normative)

Description of the SGERG-88 method

This annex gives the equations for and numerical values of coefficients which together specify completely the SGERG method for calculation of compression factors.

It also describes iteration procedures adopted by GERG [3] for implementing the method in the verified Fortran 77 subroutine SGERG.FOR. This subroutine provides the correct solution; other computational procedures are acceptable provided that they can be demonstrated to yield identical numerical results. The calculated results shall agree to at least the fourth place of decimals with the examples given in annex C.

Other implementations which are known to produce identical results are as follows:

- a) A Basic version, described in GERG TMS [3], which may be used with a variety of metric reference conditions. This programme was designed mainly for PC applications.
- b) A version in C, described in German DVGW Directives, sheet G486 [8].
- c) A version in Turbo Pascal.

All these programmes have been verified to give the same results to within 10^{-5} . The availability of the programmes and the conditions which apply to their use are discussed in part 1 of this International Standard.

B.1 Basic structure of the calculation method

As described in 4.2, the calculation proceeds in three steps, which are shown schematically in figure B.1.

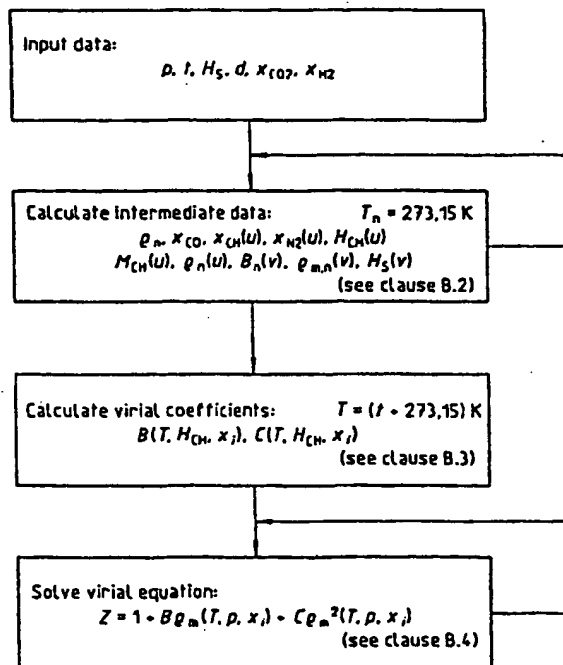


Figure B.1 — Flow diagram for standard GERG-88 calculation method
(x_i = mole fraction of component i)

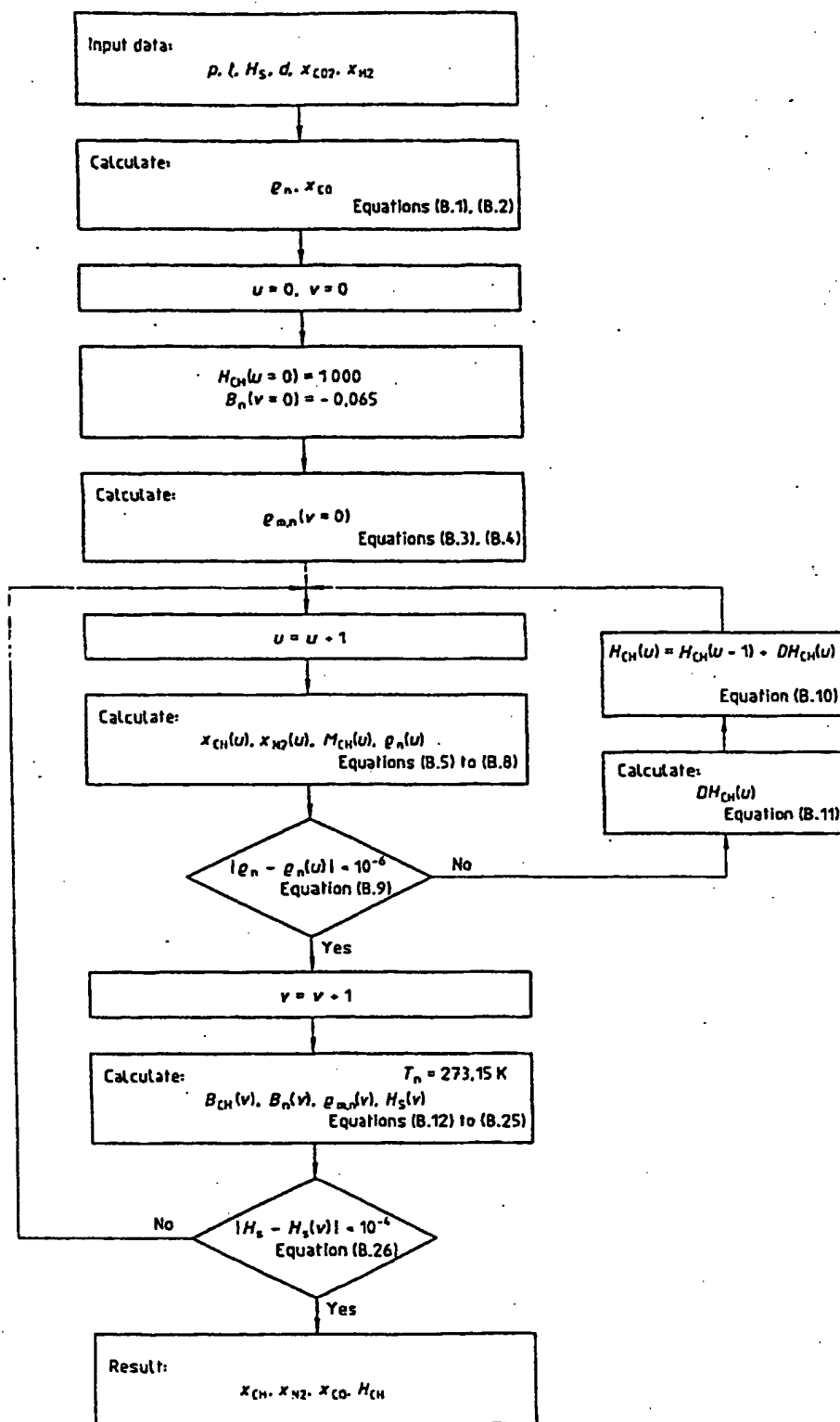


Figure B.2 — Flow diagram for computing intermediate data by iteration

$$M_{CH}(u) = -2,709\,328 + 0,021\,062\,199\,H_{CH}(u-1) \quad \dots (B.5)$$

$$x_{CH}(u) = H_S / [H_{CH}(u-1) \rho_{m,n}(v)] - [(x_{H_2} H_{H_2} + x_{CO} H_{CO}) / H_{CH}(u-1)] \quad \dots (B.6)$$

$$x_{N_2}(u) = 1 - x_{CH}(u) - x_{CO_2} - x_{H_2} - x_{CO} \quad \dots (B.7)$$

$$\rho_n(u) = [x_{CH}(u) M_{CH}(u) + x_{N_2}(u) M_{N_2}] \rho_{m,n}(v) + (x_{CO_2} M_{CO_2} + x_{H_2} M_{H_2} + x_{CO} M_{CO}) \rho_{m,n}(v) \quad \dots (B.8)$$

Table B.1 — Values of the constants used in equation (B.1)
(adjusted to conform with the molar masses and molar calorific values in ISO 6976:1975)

| | | |
|---------------|---------------|---|
| H_{H_2} | = 285,83 | MJ·kmol ⁻¹ |
| H_{CO} | = 282,98 | MJ·kmol ⁻¹ |
| M_{N_2} | = 28,013 5 | kg·kmol ⁻¹ |
| M_{CO_2} | = 44,010 | kg·kmol ⁻¹ |
| M_{H_2} | = 2,015 9 | kg·kmol ⁻¹ |
| M_{CO} | = 28,010 | kg·kmol ⁻¹ |
| R | = 0,083 145 1 | m ³ ·bar·kmol ⁻¹ ·K ⁻¹ |
| $V_{m,n}(id)$ | = 22,414 097 | m ³ ·kmol ⁻¹ |
| $\rho_n(air)$ | = 1,292 923 | kg·m ⁻³ |

B.2.1 Iteration with the molar heating value H_{CH} (inner loop)

Equations (B.1) to (B.8) are applied in sequence so as to obtain the first approximation in the u th iteration step. The starting values are:

$$H_{CH}(u=0) = 1\,000 \text{ MJ·kmol}^{-1}$$

$$B_n(v=0) = -0,065 \text{ m}^3\text{·kmol}^{-1}$$

The values of the other constants used in equations (B.1) to (B.8) are given in table B.1.

The convergence criterion for this inner iteration loop is that the absolute difference between the calculated density of the gas at normal conditions $\rho_n(u)$ and the known density (either measured directly or determined from the relative density) of the gas at normal conditions ρ_n is less than 10^{-6} , i.e.

$$|\rho_n - \rho_n(u)| < 10^{-6} \quad \dots (B.9)$$

If this condition is not satisfied, then an improved value of the molar heating value $H_{CH}(u)$, for use in equations (B.5) to (B.8), is calculated using equation (B.10) as follows:

$$H_{CH}(u) = H_{CH}(u-1) + DH_{CH}(u) \quad \dots (B.10)$$

where

$$DH_{CH}(u) = [\rho_n - \rho_n(u)] [\rho(D) - \rho_n(u)]^{-1} \quad \dots (B.11)$$

$\rho_n(u)$ being the density value for the current iteration step [commencing with $H_{CH}(u-1)$],

$\rho(D)$ being the density determined by equations (B.4) to (B.8) using $[H_{CH}(u-1) + 1]$ as input for the molar heating value.

When the left-hand side of equation (B.9) is less than 10^{-6} , this iteration loop is terminated and iteration with the second virial coefficient begins.

B.2.2 Iteration with the second virial coefficient B_n (outer loop)

The intermediate values $x_{CH}(u)$, $x_{N_2}(u)$, x_{CO} and $H_{CH}(u)$ from the preceding iteration and the input data x_{CO_2} and x_{H_2} are used to determine an improved value for the second virial coefficient $B_n(v)$ for the whole gas at normal conditions.

The second virial coefficient for the natural gas is given by the following equation:

$$B(T) = x_1^2 B_{11} + 2x_1x_2 B_{12} + 2x_1x_3 B_{13} + 2x_1x_4 B_{14} + 2x_1x_5 B_{15} + x_2^2 B_{22} + 2x_2x_3 B_{23} + 2x_2x_4 B_{24} + \\ + x_3^2 B_{33} + x_4^2 B_{44} + x_5^2 B_{55} \quad \dots (B.12)$$

Some of the terms that are missing in equation (B.12), i.e. B_{25} , B_{34} , etc., have been found not to improve the accuracy of the calculation if included and are therefore set at zero.

$$B_n(v) = B(T_n) \quad \dots (B.13)$$

where

$$T = T_n = 273,15 \quad \dots (B.14)$$

$$x_1 = x_{CH}(u) \quad \dots (B.15)$$

$$x_2 = x_{N_2}(u) \quad \dots (B.16)$$

$$x_3 = x_{CO_2} \quad \dots (B.17)$$

$$x_4 = x_{H_2} \quad \dots (B.18)$$

$$x_5 = x_{CO} \quad \dots (B.19)$$

$$B_{11} = b_{H0} + b_{H1}H_{CH}(u) + b_{H2}H_{CH}^2(u) \quad \dots (B.20)$$

where the coefficients b_{H0} , b_{H1} and b_{H2} are second-degree polynomials as a function of temperature

$$B_{11} = b_{H0}(0) + b_{H0}(1)T + b_{H0}(2)T^2 + [b_{H1}(0) + b_{H1}(1)T + b_{H1}(2)T^2]H_{CH}(u) + \\ + [b_{H2}(0) + b_{H2}(1)T + b_{H2}(2)T^2]H_{CH}^2(u) \quad \dots (B.21)$$

and the second virial coefficients B_{14} , B_{15} , B_{22} , B_{23} , B_{24} , B_{33} , B_{34} , B_{44} and B_{55} are also second-degree polynomials as a function of temperature, in the general form

$$B_{ij} = b_{ij}(0) + b_{ij}(1)T + b_{ij}(2)T^2 \quad \dots (B.22)$$

The unlike-interaction virial coefficients B_{12} and B_{13} are given by

$$B_{12} = [0,72 + 1,875 \times 10^{-5}(320 - T)^2] (B_{11} + B_{22})/2 \quad \dots (B.23)$$

$$B_{13} = -0,865(B_{11}B_{33})^{1/2} \quad \dots (B.24)$$

The coefficients in equations (B.21) to (B.24) are given in table B.2.

Table B.2 — Numerical values for the coefficients $b(0)$, $b(1)$ and $b(2)$ in the temperature expansion of the second virial coefficient for pure gases and of the unlike-interaction virial coefficients
(The units of B are $\text{m}^3\text{-kmol}^{-1}$ when the temperature is in kelvins)

| | ij | $b(0)$ | $b(1)$ | $b(2)$ |
|----------------------------------|------|--|-----------------------------|------------------------------|
| CH | H0 | $-4,254\ 68 \times 10^{-1}$ | $-2,865\ 00 \times 10^{-3}$ | $-4,620\ 73 \times 10^{-6}$ |
| CH | H1 | $8,771\ 18 \times 10^{-4}$ | $-5,562\ 81 \times 10^{-6}$ | $8,815\ 10 \times 10^{-9}$ |
| CH | H2 | $-8,247\ 47 \times 10^{-7}$ | $4,314\ 36 \times 10^{-9}$ | $-6,083\ 19 \times 10^{-12}$ |
| N ₂ | 22 | $-1,446\ 00 \times 10^{-1}$ | $7,409\ 10 \times 10^{-4}$ | $-9,119\ 50 \times 10^{-7}$ |
| CO ₂ | 33 | $-8,683\ 40 \times 10^{-1}$ | $4,037\ 60 \times 10^{-3}$ | $-5,165\ 70 \times 10^{-6}$ |
| H ₂ | 44 | $-1,105\ 96 \times 10^{-3}$ | $8,133\ 85 \times 10^{-5}$ | $-9,872\ 20 \times 10^{-8}$ |
| CO | 55 | $-1,308\ 20 \times 10^{-1}$ | $6,025\ 40 \times 10^{-4}$ | $-6,443\ 00 \times 10^{-7}$ |
| CH + N ₂ | 12 | $y = 0,72 + 1,875 \times 10^{-5}(320 - T)^2$ | | |
| CH + CO ₂ | 13 | $y = -0,865$ | | |
| CH + H ₂ | 14 | $-5,212\ 80 \times 10^{-2}$ | $2,715\ 70 \times 10^{-4}$ | $-2,500\ 00 \times 10^{-7}$ |
| CH + CO | 15 | $-6,872\ 90 \times 10^{-2}$ | $-2,393\ 81 \times 10^{-6}$ | $5,181\ 95 \times 10^{-7}$ |
| N ₂ + CO ₂ | 23 | $-3,396\ 93 \times 10^{-1}$ | $1,611\ 76 \times 10^{-3}$ | $-2,044\ 29 \times 10^{-6}$ |
| N ₂ + H ₂ | 24 | $1,200\ 00 \times 10^{-2}$ | $0,000\ 00$ | $0,000\ 00$ |

The value of $B_n(v)$ obtained from equation (B.13) is used to calculate the v th approximation of $\rho_{m,n}$ using equation (B.4).

Equation (B.6) is then used, in the inverse way to that in which it was used previously, to obtain a value for $H_S(v)$, i.e.

$$H_S(v) = [x_1(u)H_{CH}(u-1) + x_4H_4 + x_5H_5]\rho_{m,n}(v) \quad \dots (B.25)$$

where $H_4 (= H_{H_2})$ and $H_5 (= H_{CO})$ are the molar heating values at 298,15 K of hydrogen and carbon monoxide, respectively. The convergence criterion for the outer iteration loop (iteration counter v) is that the absolute difference between the measured superior calorific value H_S and the calculated calorific value $H_S(v)$ is less than 10^{-4} , i.e.

$$|H_S - H_S(v)| < 10^{-4} \quad \dots (B.26)$$

If this criterion is not satisfied, then the value for $B_n(v)$ determined from equation (B.13) is used as a new input value for equation (B.4) and the whole iteration procedure, i.e. the inner iteration loop (iteration counter u), is restarted from equation (B.5) using the current values of $H_{CH}(u-1)$ and $\rho_{m,n}(v)$.

When both convergence criterion (B.9) and convergence criterion (B.26) are satisfied simultaneously, the final intermediate data for the mole fractions x_{CH} and x_{N_2} and for the molar heating value H_{CH} have been determined.

B.3 Calculation of virial coefficients

The second and third virial coefficients $B(T)$ and $C(T)$ of a natural gas are now determined from the mole fractions x_{CO_2} and x_{H_2} (input data) and x_{CH} , x_{N_2} and x_{CO} (intermediate data) and the molar heating value H_{CH} (see figures B.1 and B.3).

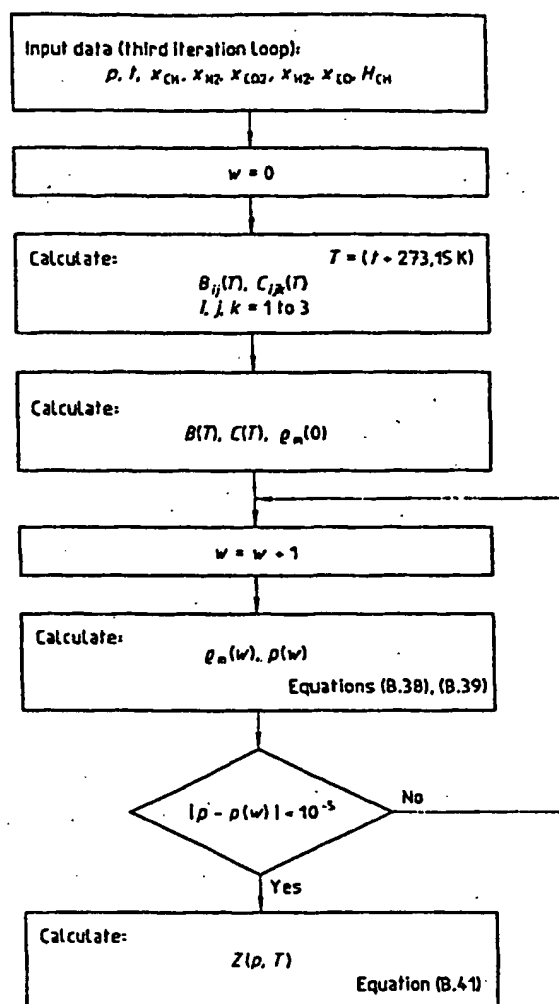


Figure B.3 — Flow diagram for compression factor calculation

B.3.1 Calculation of $B(T)$

The second virial coefficient $B(T)$ is calculated from equation (B.12) by the procedure described in B.2.2 for a temperature

$$T = t + 273,15 \quad \dots (B.27)$$

B.3.2 Calculation of $C(T)$

The third virial coefficient for a natural gas at a temperature T is determined using the following equation:

$$\begin{aligned}
 C(T) = & x_1^3 C_{111} + 3x_1^2 x_2 C_{112} + 3x_1^2 x_3 C_{113} + 3x_1^2 x_4 C_{114} + 3x_1^2 x_5 C_{115} + 3x_1 x_2^2 C_{122} + 6x_1 x_2 x_3 C_{123} + \\
 & + 3x_1 x_3^2 C_{133} + x_2^3 C_{222} + 3x_2^2 x_3 C_{223} + 3x_2 x_3^2 C_{233} + x_3^3 C_{333} + x_4^3 C_{444} \quad \dots (B.28)
 \end{aligned}$$

The possible additional terms that are missing in equation (B.28) have been found not to improve the accuracy of the calculation if included and have therefore been set at zero.

Furthermore, in equation (B.28):

$$C_{111} = c_{H0} + c_{H1}H_{CH} + c_{H2}H_{CH}^2 \quad \dots (B.29)$$

where c_{H0} , c_{H1} and c_{H2} are second-degree polynomials as a function of temperature, viz:

$$C_{111} = c_{H0}(0) + c_{H0}(1)T + c_{H0}(2)T^2 + [c_{H1}(0) + c_{H1}(1)T + c_{H1}(2)T^2]H_{CH} + [c_{H2}(0) + c_{H2}(1)T + c_{H2}(2)T^2]H_{CH}^2 \quad \dots (B.30)$$

as are C_{222} , C_{333} , C_{444} , C_{115} , C_{223} and C_{233} , viz:

$$C_{ijk} = c_{ijk}(0) + c_{ijk}(1)T + c_{ijk}(2)T^2 \quad \dots (B.31)$$

The coefficients in equations (B.30) and (B.31) are given in table B.3.

Table B.3 — Numerical values of the coefficients $c(0)$, $c(1)$ and $c(2)$ in the temperature expansion of the third virial coefficient for pure gases and of the unlike-interaction virial coefficients
(The units of C are $m^6 \cdot kmol^{-2}$ when the temperature is in kelvins)

| | <i>ijk</i> | <i>c</i> (0) | <i>c</i> (1) | <i>c</i> (2) |
|--|------------|---------------------------------|-----------------------------|------------------------------|
| CH | H0 | $-3,024\ 88 \times 10^{-1}$ | $1,958\ 61 \times 10^{-3}$ | $-3,163\ 02 \times 10^{-6}$ |
| CH | H1 | $6,464\ 22 \times 10^{-4}$ | $-4,228\ 76 \times 10^{-6}$ | $6,881\ 57 \times 10^{-9}$ |
| CH | H2 | $-3,328\ 05 \times 10^{-7}$ | $2,231\ 60 \times 10^{-9}$ | $-3,677\ 13 \times 10^{-12}$ |
| N ₂ | 222 | $7,849\ 80 \times 10^{-3}$ | $-3,989\ 50 \times 10^{-5}$ | $6,118\ 70 \times 10^{-8}$ |
| CO ₂ | 333 | $2,051\ 30 \times 10^{-1}$ | $3,488\ 80 \times 10^{-5}$ | $-8,370\ 30 \times 10^{-8}$ |
| H ₂ | 444 | $1,047\ 11 \times 10^{-3}$ | $-3,648\ 87 \times 10^{-6}$ | $4,670\ 95 \times 10^{-9}$ |
| CH + CH + N ₂ | 112 | $y = 0,92 + 0,001\ 3 (T - 270)$ | | |
| CH + CH + CO ₂ | 113 | $y = 0,92$ | | |
| CH + CH + H ₂ | 114 | $y = 1,20$ | | |
| CH + CH + CO | 115 | $-7,367\ 48 \times 10^{-3}$ | $-2,765\ 78 \times 10^{-5}$ | $3,430\ 51 \times 10^{-8}$ |
| CH + N ₂ + N ₂ | 122 | $y = 0,92 + 0,001\ 3 (T - 270)$ | | |
| CH + N ₂ + CO ₂ | 123 | $y = 1,10$ | | |
| CH + CO ₂ + CO ₂ | 133 | $y = 0,92$ | | |
| N ₂ + N ₂ + CO ₂ | 223 | $5,520\ 66 \times 10^{-3}$ | $-1,686\ 09 \times 10^{-5}$ | $1,571\ 69 \times 10^{-8}$ |
| N ₂ + CO ₂ + CO ₂ | 233 | $3,587\ 83 \times 10^{-3}$ | $8,066\ 74 \times 10^{-6}$ | $-3,257\ 98 \times 10^{-8}$ |

The other unlike-interaction virial coefficients used are given by

$$C_{ijk} = y_{ijk} (C_{iii} C_{jjj} C_{kkk})^{1/3} \quad \dots (B.32)$$

where y_{ijk} is given by

$$y_{112} = y_{122} = 0,92 + 0,001\ 3(T - 270) \quad \dots (B.33)$$

$$y_{113} = y_{133} = 0,92 \quad \dots (B.34)$$

$$y_{114} = 1,20 \quad \dots (B.35)$$

$$y_{123} = 1,10 \quad \dots (B.36)$$

Equation (B.32) shows that the temperature dependence of the unlike-interaction virial coefficients is determined essentially by the temperature dependence of the third virial coefficients for the pure components.

B.4 Calculation of the compression factor and molar density

The very last stage in the calculation of the compression factor and the molar density is to solve equations (1) and (2) simultaneously for the given value of the pressure p . For the first approximation in the iteration using w , ρ_m is given by

$$\rho_m^{-1}(w=0) = RT/p + B \quad \dots (B.37)$$

where the second virial coefficient B is defined by equation (B.12) for a temperature T (see figure B.3). An improved value $\rho_m(w)$ is then given by

$$\rho_m^{-1}(w) = (RT/p) [1 + B\rho_m(w-1) + C\rho_m^2(w-1)] \quad \dots (B.38)$$

where the third virial coefficient C for the mixture is defined by equation (B.28) for a given temperature T . The convergence criterion for the iteration using w is that the absolute difference between the calculated pressure $p(w)$ given by equation (B.39) and the given pressure p is less than 10^{-5} [see equation (B.40)].

$$p(w) = RT\rho_m(w) [1 + B\rho_m(w) + C\rho_m^2(w)] \quad \dots (B.39)$$

$$|p - p(w)| < 10^{-5} \quad \dots (B.40)$$

If this condition is not satisfied, then the current value for the molar density $\rho_m(w)$ is used as the new value $\rho_m(w-1)$ in equation (B.38) and an improved value of the molar density $\rho_m(w)$ is calculated.

However, if the left-hand side of equation (B.40) is less than 10^{-5} , the iteration routine is ended, and $\rho_m(w)$ is the final molar density ρ_m . The compression factor is then given by

$$Z = 1 + B\rho_m + C\rho_m^2 \quad \dots (B.41)$$

NOTE — The mass density can be calculated as follows:

$$\rho = [d\rho_n(\text{air})pZ_nT_n / (p_nZT)] \quad \dots (B.42)$$

Z and Z_n being rounded to four places of decimals before being used in the density calculation.

Report the density to 3 significant figures.

B.5 Consistency checks on the SGERG-88 method

The following tests, which provide partial consistency checks on the input data, shall be applied when carrying out calculations by the SGERG method.

a) The input data shall satisfy the following condition:

$$d > 0,55 + 0,97x_{\text{CO}_2} - 0,45x_{\text{H}_2} \quad \dots (B.43)$$

b) The intermediate calculated value for the mole fraction of nitrogen shall satisfy the following conditions:

$$-0,01 \leq x_{\text{N}_2} \leq 0,5 \quad \dots (B.44)$$

$$x_{\text{N}_2} + x_{\text{CO}_2} \leq 0,5 \quad \dots (B.45)$$

c) Furthermore, the internal consistency of the input data for the third iteration loop shall satisfy the condition:

$$d > 0,55 + 0,4x_{\text{N}_2} + 0,97x_{\text{CO}_2} - 0,45x_{\text{H}_2} \quad \dots (B.46)$$

Annex C (normative)

Example calculations

The following example calculations shall be used for the validation of computer implementations of the SGERG method not cited in annex B. The calculations have been carried out using the validated executable programme GERG88.EXE, which incorporates the subroutine SGERG.FOR described in annex B.

Table C.1 — Input data

| | Gas 1 | Gas 2 | Gas 3 | Gas 4 | Gas 5 | Gas 6 |
|-----------------------------|-------|-------|-------|-------|-------|-------|
| x_{CO_2} | 0,006 | 0,005 | 0,015 | 0,016 | 0,076 | 0,011 |
| x_{H_2} | 0,000 | 0,000 | 0,000 | 0,095 | 0,000 | 0,000 |
| d | 0,581 | 0,609 | 0,650 | 0,599 | 0,686 | 0,644 |
| H_S (MJ·m ⁻³) | 40,66 | 40,62 | 43,53 | 34,16 | 36,64 | 36,58 |

Table C.2 — Results (Z-values)

| Conditions | | Gas 1 | Gas 2 | Gas 3 | Gas 4 | Gas 5 | Gas 6 |
|------------|-----------|----------|----------|----------|----------|----------|----------|
| p bar | t °C | | | | | | |
| 60 | -3,15 | 0,840 84 | 0,833 97 | 0,794 15 | 0,885 69 | 0,826 64 | 0,854 06 |
| 60 | 6,85 | 0,862 02 | 0,856 15 | 0,822 10 | 0,901 50 | 0,850 17 | 0,873 88 |
| 60 | 16,85 | 0,880 07 | 0,875 00 | 0,845 53 | 0,915 07 | 0,870 03 | 0,890 71 |
| 60 | 36,85 | 0,908 81 | 0,904 91 | 0,882 23 | 0,936 84 | 0,901 24 | 0,917 36 |
| 60 | 56,85 | 0,929 96 | 0,926 90 | 0,908 93 | 0,953 02 | 0,923 94 | 0,936 90 |
| 120 | -3,15 | 0,721 46 | 0,711 40 | 0,643 22 | 0,808 43 | 0,695 57 | 0,749 39 |
| 120 | 6,85 | 0,759 69 | 0,750 79 | 0,690 62 | 0,836 13 | 0,738 28 | 0,784 73 |
| 120 | 16,85 | 0,792 57 | 0,784 72 | 0,731 96 | 0,859 99 | 0,774 63 | 0,814 90 |
| 120 | 36,85 | 0,844 92 | 0,838 77 | 0,797 78 | 0,898 27 | 0,831 66 | 0,862 66 |
| 120 | 56,85 | 0,883 22 | 0,878 32 | 0,845 54 | 0,926 62 | 0,872 69 | 0,897 49 |

These gases are the same as the six gases in ISO 12213-2, annex C, where the complete molar compositions are given.

Annex D (normative)

Conversion factors

D.1 Reference conditions

The reference conditions for which the standard GERG-88 virial equation was developed and which the SGERG.FOR computer subroutine uses internally are

Calorific value by combustion at $T_1 = 298,15 \text{ K}$ ($t_1 = 25 \text{ °C}$)
 $p = 101,325 \text{ kPa}$

gas metered at $T_2 = 273,15 \text{ K}$ ($t_2 = 0 \text{ °C}$)
 $p = 101,325 \text{ kPa}$

The latter set of conditions are also the reference conditions for relative density.

Considerable care is needed to ensure that correctly referenced inputs are used for calorific value and relative density. Several countries normally use the above conditions, but others use alternative conditions. This can easily cause confusion, particularly since the unit of calorific-value measurement in each case may still be $\text{MJ}\cdot\text{m}^{-3}$. Table D.1 is a guide to which of the major international gas-trading countries use which reference conditions.

For those using non-metric units for calorific value (i.e. $\text{Btu}\cdot\text{ft}^{-3}$), conversion both of units and of reference conditions is required.

The conversion factors used are taken from reference [3].

Table D.1 — Nationally adopted metric reference conditions for the measurement of calorific value

| | t_1 (°C) | t_2 (°C) |
|--|------------|------------|
| Australia | 15 | 15 |
| Austria | 25 | 0 |
| Belgium | 25 | 0 |
| Canada | 15 | 15 |
| Denmark | 25 | 0 |
| France | 0 | 0 |
| Germany | 25 | 0 |
| Ireland | 15 | 15 |
| Italy | 25 | 0 |
| Japan | 0 | 0 |
| Netherlands | 25 | 0 |
| Russia | 25 | 0 or 20 |
| United Kingdom | 15 | 15 |
| United States of America | 15 | 15 |
| NOTES | | |
| 1 In all countries the reference pressure is 101,325 kPa (= 1,013 25 bar). | | |
| 2 t_1 is the combustion reference temperature. | | |
| 3 t_2 is the gas-metering reference temperature. | | |

D.2 Units and conversion factors for pressure and temperature

If the input variables p and t are not in the necessary units of bar and °C, then conversions must be made in order to use the Fortran implementation. A selection of appropriate conversion factors is given in table D.2.

Table D.2 — Conversion factors for pressure and temperature

| | |
|--------------------|--|
| Pressure | |
| p (bar) | $= [p(\text{kPa})]/100$ |
| p (bar) | $= [p(\text{MPa})] \times 10$ |
| p (bar) | $= [p(\text{atm})] \times 1,013\,25$ |
| p (bar) | $= [p(\text{psia})]/14,503\,8$ |
| p (bar) | $= [p(\text{psig}) + 14,695\,9]/14,503\,8$ |
| Temperature | |
| t (°C) | $= T(\text{K}) - 273,15$ |
| t (°C) | $= [t(°\text{F}) - 32]/1,8$ |
| t (°C) | $= [t(°\text{R})]/1,8 - 273,15$ |

D.3 Units and conversion of calorific value and density between reference conditions

Because both superior calorific value and relative density are functions of the composition of a gas mixture, and because the thermophysical properties of the individual components depend upon temperature and pressure in individual ways, it is in principle impossible (without knowledge of the composition) to convert the calorific value and the relative density, known at one set of reference conditions, to exact corresponding values for any other set of reference conditions.

However, because the relevant reference conditions are always thermodynamically close together, and because natural gases do not vary in their composition to any major extent, it is possible in practice to give conversion factors which may be applied to any typical natural gas with essentially no loss of accuracy in the converted physical properties.

D.3.1 Conversion factors for the units

If the input variable H_S is not in the necessary units MJ·m⁻³, then a conversion must be made.

The appropriate conversion factors for calorific values at a given set of reference conditions (see clause D.1) are given in table D.3.

Table D.3 — Conversion factors for calorific value

| | |
|-----------------------------|---|
| H_S (MJ·m ⁻³) | $= [H_S(\text{kWh·m}^{-3})] \times 3,6$ |
| H_S (MJ·m ⁻³) | $= [H_S(\text{Btu·ft}^{-3})]/26,839\,2$ |

D.3.2 Conversion between different reference conditions

If the input variables H_S and d are not at the correct reference conditions (see clause D.1), then a conversion must be made. Table D.4 gives the conversion factors appropriate to the reference conditions in table D.1.

Table D.4 — Conversion factors for calorific value and relative density

| |
|--|
| <p>Calorific value H_S at reference conditions</p> <p>$t_1 = 25\text{ °C}, t_2 = 0\text{ °C}, p_2 = 1,013\ 25\text{ bar}$:</p> <p>$H_S = H_S(t_1 = 0\text{ °C}, t_2 = 0\text{ °C}, p_2 = 1,013\ 25\text{ bar}) \times 0,997\ 4$</p> <p>$H_S = H_S(t_1 = 15\text{ °C}, t_2 = 15\text{ °C}, p_2 = 1,013\ 25\text{ bar}) \times 1,054\ 3$</p> <p>$H_S = H_S(t_1 = 60\text{ °F}, t_2 = 60\text{ °F}, p_2 = 1,015\ 92\text{ bar}) \times 1,053\ 5$</p> <p>$H_S = H_S(t_1 = 60\text{ °F}, t_2 = 60\text{ °F}, p_2 = 1,015\ 60\text{ bar}) \times 1,053\ 9$</p> |
| <p>Relative density d at reference conditions</p> <p>$t_2 = 0\text{ °C}, p_2 = 1,013\ 25\text{ bar}$:</p> <p>$d = d(t_2 = 15\text{ °C}, p_2 = 1,013\ 25\text{ bar}) \times 1,000\ 2$</p> <p>$d = d(t_2 = 60\text{ °F}, p_2 = 1,015\ 92\text{ bar or } 1,015\ 60\text{ bar}) \times 1,000\ 2$</p> |
| <p>NOTE — $p = 1,015\ 60\text{ bar} = 14,73\text{ psia}$ (pressure customary in US).</p> |

Annex E (informative)

Performance over wider ranges of application

The standard GERG virial equation has been comprehensively tested, over the temperature range 263 K to 338 K and at pressures up to 12 MPa, with the GERG databank [5] and the Gas Research Institute data [9] for gases within the ranges of composition, superior calorific value and relative density given for pipeline quality gases (see 4.4.1). Within these limits, the uncertainties are as given in 4.5.

Rough estimates of the uncertainties involved in calculations of compression factors for wider ranges of application are plotted in figures E.1 to E.4 as pressure-composition plots for nitrogen, carbon dioxide, ethane and propane, respectively.

In figures E.1 to E.4, the performance of the SGERG equation is illustrated up to a maximum pressure of 30 MPa. This is for informative purposes only and is not intended to imply a recommendation that the equation be used routinely or uncritically above the normal specified limits. The uncertainty limits are dependent upon pressure, temperature and composition, and are also strongly affected by the proximity of the phase boundary. The estimated uncertainty limits presented below are based upon less comprehensive data, published as a supplement to the GERG databank [6], and upon the databanks in references [5] and [9].

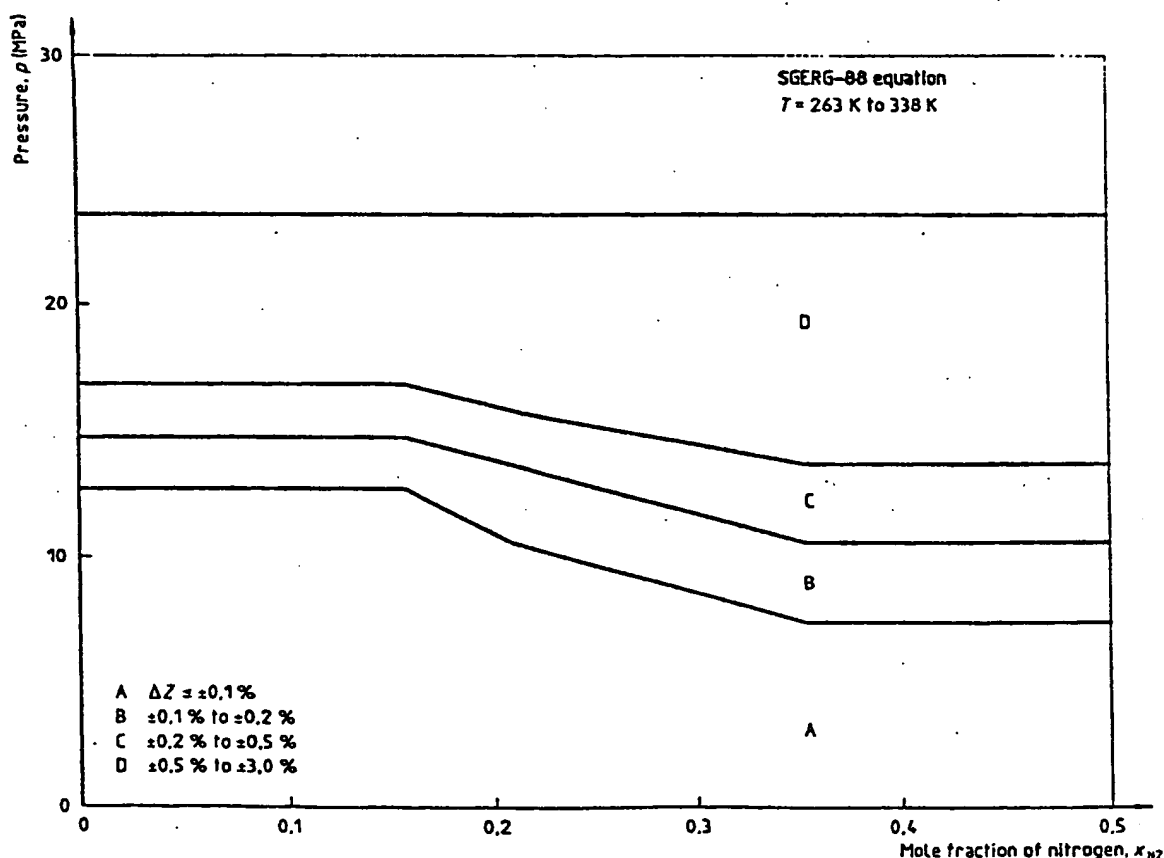


Figure E.1 — Estimated uncertainty limits for the calculation of compression factors of natural gases with a high nitrogen content

The worst-case limits have always been chosen. Dashed lines are used to separate two regions of estimated uncertainty when the experimental evidence is not sufficient to determine the position of the boundary. The detailed composition of the gas will have a strong influence on the position of the phase boundary and the user should, therefore, make his own phase boundary calculation.

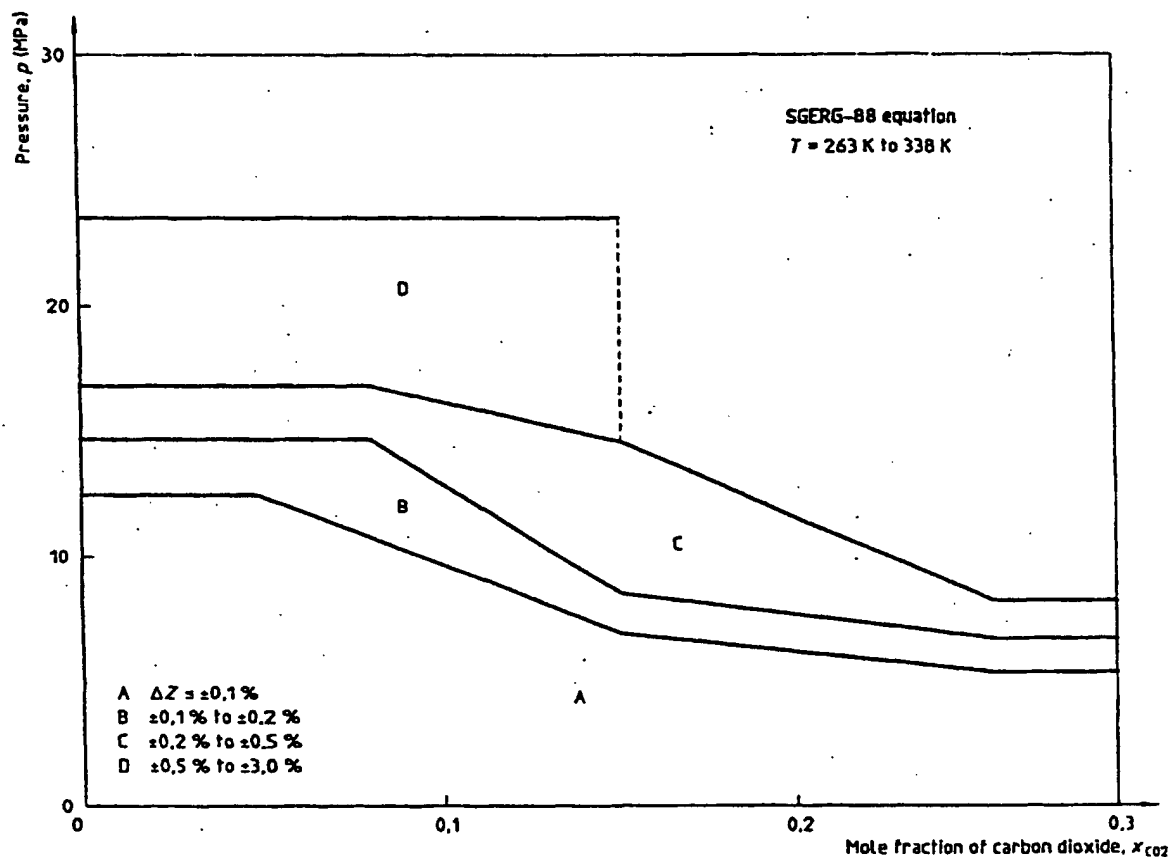


Figure E.2 — Estimated uncertainty limits for the calculation of compression factors of natural gases with a high carbon dioxide content

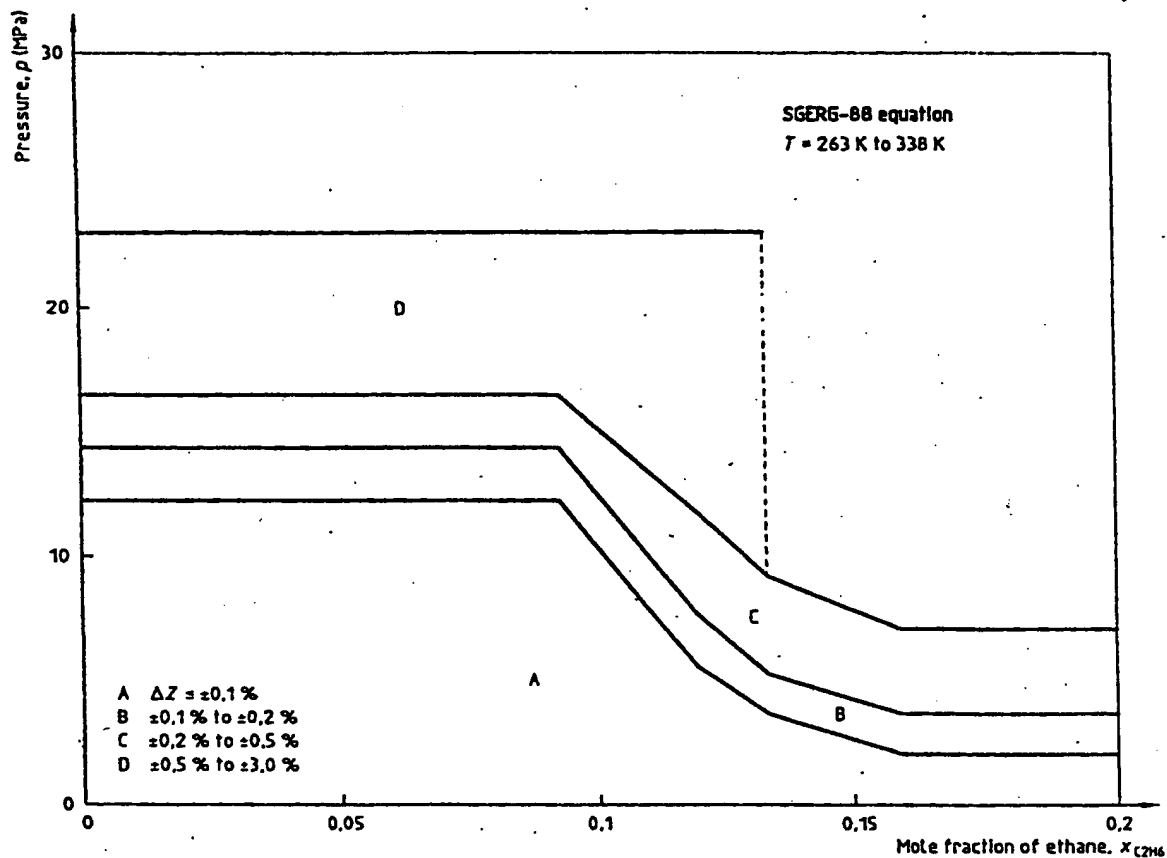


Figure E.3 — Estimated uncertainty limits for the calculation of compression factors of natural gases with a high ethane content

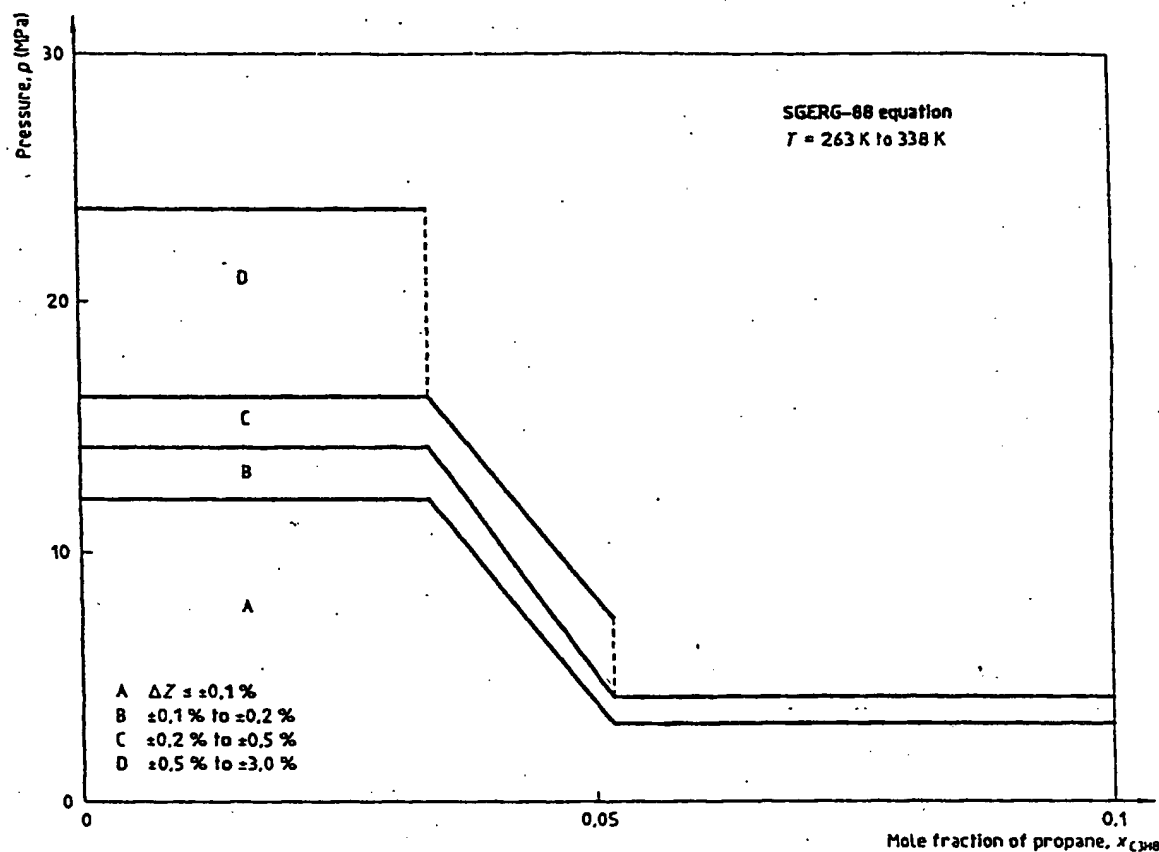


Figure E.4 — Estimated uncertainty limits for the calculation of compression factors of natural gases with a high propane content

The overall results at pressures up to 10 MPa and temperatures within the range 263 K to 338 K can be summarized as follows. Only gases having mole fractions within the limits given below will have uncertainties within $\pm 0,1 \%$, $\pm 0,2 \%$ and $\pm 0,5 \%$, respectively, within the given pressure and temperature domain.

| Component | Mole fraction for an uncertainty within | | |
|----------------|---|--------------|--------------|
| | $\pm 0,1 \%$ | $\pm 0,2 \%$ | $\pm 0,5 \%$ |
| Nitrogen | $\leq 0,20$ | $\leq 0,50$ | — |
| Carbon dioxide | $\leq 0,09$ | $\leq 0,12$ | $\leq 0,23$ |
| Ethane | $\leq 0,10$ | $\leq 0,11$ | $\leq 0,12$ |
| Propane | $\leq 0,035$ | $\leq 0,04$ | $\leq 0,045$ |

Annex F (informative)

Subroutine SGERG.FOR in Fortran

```

C*****
C last update: 07.08.96                      M. Jaeschke, J. Sikora
C*****
C      GERG-88 VIRIAL EQUATION *****
C      SUBROUTINE SGERG
C
C      'SGERG'    CALCULATES THE COMPRESSION FACTORS OF NATURAL GASES USING
C                  A SIMPLIFIED GAS ANALYSIS
C
C      LEGAL COPIES OF THIS PROGRAM MAY ONLY BE OBTAINED FROM THE
C      MEMBERS OF THE GERG WORKING GROUP ON COMPRESSION
C      FACTORS OF NATURAL GAS AS GIVEN IN THE GERG TECHNICAL
C      MONOGRAPH TM 5 (1991).
C
C      The calculations are based on the following four
C      input parameters for the gas analysis:
C
C      (Valid ranges:)
C      -1- X3: mole fraction CO2                ( 0.0 -> 0.3 )
C      -2- HS: calorific value in MJ/m^3 *)      ( 20 -> 48 )
C      -3- RM: relative density                  ( 0.55 -> 0.9 )
C      -4- X5: mole fraction H2                  ( 0.0 -> 0.1 )
C
C      *) note : metering at T = 0.0 C , P = 1.01325 bar
C                  : combustion at T = 25.0 C
C
C      Further input parameters used are:
C
C      P : pressure in bar                      ( 0 -> 120 )
C      TC: temperature in degrees Celsius      (-23 -> 65 )
C
C      A CALCULATED value for X2, the molar fraction of nitrogen
C      is returned.
C
C      The calculated values are:
C
C      Z : compression factor
C      D : molar density in mol/m**3
C
C      **** For some compilers the SAVE option has to be set explicitly ****
C
C      SYNTAX :    CALL SGERG(X2,X3,HS,RM,X5,P,TC,Z,D)
C
C      The coefficients used in this program are conform with the
C      values given in subroutine GAS682, from July 20,1988, appended
C      to report 8807, Van der Waals Laboratory, Amsterdam.
C
C      J.P.J. Michels & J.A. Schouten
C      August 16, 1991
C
C      Values for the gas constant, molar masses, calorific values
C      and the density of air conform with ISO 6976 (1995).
C
C*****
C
C      SUBROUTINE SGERG(X2,X3,HS,RM,X5,P,TC,Z,D)
C      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C      IF( P.LT. 0.0 .OR. P.GT.120.0) STOP ' PRESSURE OUT OF RANGE'
C      IF(TC.LT.-23.0 .OR. TC.GT.65.0) STOP ' TEMPERATURE OUT OF RANGE'
C      CALL SGERG1(P,TC,X2,X3,X5,HS,RM,Z,D)
C      RETURN
C      END

```

```

C *****
SUBROUTINE SGERG1(P,TC,Q2,Q3,Q5,QM,RM,Z,D)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
COMMON /RBLOK/ AMOL,HS
COMMON /XBLOK/ X1,X2,X3,X11,X12,X13,X22,X23,X33
> ,X5,X7,X15,X17,X25,X55,X77
COMMON /MBLOK/ GM1R0,GM1R1,GM2,GM3,GM5,GM7,FA,FB,RL,T0,H5,H7,R
HS = QM
X3 = Q3
X5 = Q5
C IF(RM.LT. 0.55.OR. RM.GT. 0.90) STOP 'REL. MASS OUT OF RANGE'
C IF(X3.LT. 0.0 .OR. X3.GT. 0.30) STOP 'CO2 OUT OF RANGE'
C IF(HS.LT.20.0 .OR. HS.GT.48.0 ) STOP 'CALOR. VALUE OUT OF RANGE'
IF((0.55+0.97*X3-0.45*X5).GT.RM)STOP 'CONFLICTING INPUT'
SM = RM*RL
X7 = X5*0.0964D0
X33 = X3*X3
X55 = X5*X5
X77 = X7*X7
BEFF= -0.065D0
H = 1000.0D0
AMOL= 1.0D0/(FA+BEFF)
K = 0
KK = 0
1 CALL SMBER(H,SMT1)
IF(ABS(SM-SMT1) .GT. 1.D-6) THEN
CALL SMBER(H+1.0D0,SMT2)
DH= (SM-SMT1)/(SMT2-SMT1)
H = H+DH
KK = KK+1
IF(KK.GT.20)STOP ' NO CONVERGENCY #1'
GO TO 1
END IF
X11 = X1*X1
X12 = X1*X2
X13 = X1*X3
X22 = X2*X2
X23 = X2*X3
X25 = X2*X5
X15 = X1*X5
X17 = X1*X7
CALL B11BER(T0,H,B11)
CALL BBER(T0,B11,BEFF)
AMOL= 1.0D0/(FA+BEFF)
HSBER = X1*H*AMOL+(X5*H5+X7*H7)*AMOL
IF(ABS(HS-HSBER).GT.1.0D-4) THEN
K = K+1
IF(K.GT.20)STOP 'NO CONVERGENCY #2'
GO TO 1
END IF
IF(X2.LT.-0.01 .OR. X2.GT.0.5) STOP 'CALC. N2 OUT OF RANGE'
IF(X2+X3.GT.0.5) STOP 'N2 + CO2 OUT OF RANGE'
IF(0.55+.4*X2+0.97*X3-0.45*X5).GT.RM)
+ STOP 'CONFLICTING RESULT FOR N2'
Q2 = X2
T = TC+T0
CALL B11BER(T,H,B11)
CALL BBER(T,B11,B)
CALL CBER(T,H,C)
CALL ITER(P,T,B,C,V,Z)
D = 1.0D0/V
END
SUBROUTINE SMBER(H,SM)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
COMMON /RBLOK/ AMOL,HS
COMMON /XBLOK/ X1,X2,X3,X11,X12,X13,X22,X23,X33
> ,X5,X7,X15,X17,X25,X55,X77
COMMON /MBLOK/ GM1R0,GM1R1,GM2,GM3,GM5,GM7,FA,FB,RL,T0,H5,H7,R
GM1= GM1R0+GM1R1*H
X1 = (HS-(X5*H5+X7*H7)*AMOL)/H/AMOL

```

```

X2 = 1.0D0-X1-X3-X5-X7
SM = (X1*GM1+X2*GM2+X3*GM3+X5*GM5+X7*GM7)*AMOL
END

```

C
C

```

*****
SUBROUTINE B11BER(T,H,B11)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
COMMON /BBLOK/ BR11H0(3), BR11H1(3), BR11H2(3), BR22(3), BR23(3),
+ BR33(3), BR15(3), BR17(3), BR55(3), BR77(3), B25
T2=T*T
B11=BR11H0(1) + BR11H0(2)*T + BR11H0(3)*T2
+ (BR11H1(1) + BR11H1(2)*T + BR11H1(3)*T2)*H
+ (BR11H2(1) + BR11H2(2)*T + BR11H2(3)*T2)*H*H
END

```

C

```

*****
SUBROUTINE BBER(T,B11,BEFF)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
COMMON /BBLOK/ BR11H0(3), BR11H1(3), BR11H2(3), BR22(3), BR23(3),
+ BR33(3), BR15(3), BR17(3), BR55(3), BR77(3), B25
COMMON /ZETA/ Z12,Z13,Y12,Y13,Y123,Y115
COMMON /XBLOK/ X1,X2,X3,X11,X12,X13,X22,X23,X33
+ X5,X7,X15,X17,X25,X55,X77
T2=T*T
B22=BR22(1) + BR22(2)*T + BR22(3)*T2
B23=BR23(1) + BR23(2)*T + BR23(3)*T2
B33=BR33(1) + BR33(2)*T + BR33(3)*T2
B15=BR15(1) + BR15(2)*T + BR15(3)*T2
B55=BR55(1) + BR55(2)*T + BR55(3)*T2
B17=BR17(1) + BR17(2)*T + BR17(3)*T2
B77=BR77(1) + BR77(2)*T + BR77(3)*T2
BA13= B11*B33
IF (BA13 .LT. 0.0) STOP ' NO SOLUTION'
ZZZ=Z12+(320.0D0-T)**2*1.875D-5
BEFF = X11*B11 + X12*ZZZ*(B11+B22) + 2.0D0*X13*Z13*DSQRT(BA13)
+ X22*B22 + 2.0D0*X23*B23 + X33*B33 + X55*B55
+ 2.0D0*X15*B15 + 2.0D0*X25*B25 + 2.0D0*X17*B17 + X77*B77
END

```

C

```

*****
SUBROUTINE CBER(T,H,CEFF)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
COMMON /CBLOK/ CR111H0(3), CR111H1(3), CR111H2(3), CR222(3),
+ CR223(3), CR233(3), CR333(3), CR555(3), CR117(3)
COMMON /ZETA/ Z12,Z13,Y12,Y13,Y123,Y115
COMMON /XBLOK/ X1,X2,X3,X11,X12,X13,X22,X23,X33
+ X5,X7,X15,X17,X25,X55,X77
T2=T*T
C111=CR111H0(1) + CR111H0(2)*T + CR111H0(3)*T2
+ (CR111H1(1) + CR111H1(2)*T + CR111H1(3)*T2)*H
+ (CR111H2(1) + CR111H2(2)*T + CR111H2(3)*T2)*H*H
C222 = CR222(1) + CR222(2)*T + CR222(3)*T2
C223 = CR223(1) + CR223(2)*T + CR223(3)*T2
C233 = CR233(1) + CR233(2)*T + CR233(3)*T2
C333 = CR333(1) + CR333(2)*T + CR333(3)*T2
C555 = CR555(1) + CR555(2)*T + CR555(3)*T2
C117 = CR117(1) + CR117(2)*T + CR117(3)*T2
CA112=C111*C111*C222
CA113=C111*C111*C333
CA122=C111*C222*C222
CA123=C111*C222*C333
CA133=C111*C333*C333
CA115=C111*C111*C555
IF (CA112.LT.0.0 .OR. CA113.LT.0.0 .OR. CA122.LT.0.0
+ .OR. CA123.LT.0.0 .OR. CA133.LT.0.0 .OR. CA115.LT.0.0)
+ STOP ' NO SOLUTION'
D3REP=1.0D0/3.0D0
CEFF=X1*X11*C111 + 3.0D0*X11*X2*(CA112)**D3REP*(Y12+(T-270.0D0)
+ *0.0013D0)
+ 3.0D0*X11*X3 *(CA113)**D3REP *Y13
+ 3.0D0*X1*X15 *(CA115)**D3REP *Y115
+ 3.0D0*X1*X22 *(CA122)**D3REP *(Y12+(T-270.0D0)*0.0013D0)

```

```

+      +6.0D0*X1*X2*X3*(CA123)**D3REP *Y123
+      +3.0D0*X1*X33 *(CA133)**D3REP *Y13
+      +X22*X2*C222 + 3.0D0*X22*X3*C223 + 3.0D0*X2*X33*C233
+      +X3*X33*C333 +      X5*X55*C555 + 3.0D0*X11*X7*C117
RETURN
END
C *****
SUBROUTINE ITER(P,T,B,C,V,Z)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
COMMON /MBLOK/ GM1R0,GM1R1,GM2,GM3,GM5,GM7,FA,FB,RL,T0,H5,H7,R
RT = R*T
RTP= RT/P
V = RTP+B
KK = 0
5 V = RTP*(1.0D0+B/V+C/V**2)
KK = KK+1
IF (KK.GT. 20) STOP ' NO CONVERGENCY #3'
Z = 1.0D0+B/V+C/V**2
PA = RT/V*Z
IF(ABS(PA-P) .GE. 1.D-5)GO TO 5
RETURN
END
C *****
BLOCK DATA
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
COMMON /BBLOK/ BR11H0(3), BR11H1(3), BR11H2(3), BR22(3), BR23(3),
+ BR33(3), BR15(3), BR17(3), BR55(3), BR77(3), B25
COMMON /CBLOK/ CR11H0(3), CR11H1(3), CR11H2(3), CR222(3),
+ CR223(3), CR233(3), CR333(3), CR555(3), CR117(3)
COMMON /ZETA/ Z12,Z13,Y12,Y13,Y123,Y115
COMMON /MBLOK/ GM1R0,GM1R1,GM2,GM3,GM5,GM7,FA,FB,RL,T0,H5,H7,R
DATA BR11H0/-0.425468D0, 0.286500D-2, -.462073D-5 /,
+ BR11H1/0.877118D-3, -.556281D-5, 0.881510D-8 /,
+ BR11H2/-0.824747D-6, 0.431436D-8, -.608319D-11/,
+ BR22 / -.144600D0 , 0.740910D-3, -.911950D-6 /,
+ BR23 / -.339693D0 , 0.161176D-2, -.204429D-5 /,
+ BR33 / -.868340D0 , 0.403760D-2, -.516570D-5 /,
+ BR15 / -.521280D-1, 0.271570D-3, -.25 D-6 /,
+ BR17 / -.687290D-1, -.239381D-5, 0.518195D-6 /,
+ BR55 / -.110596D-2, 0.813385D-4, -.987220D-7 /,
+ BR77 / -.130820D0 , 0.602540D-3, -.644300D-6 /,
+ B25 / 0.012D0 /
DATA CR11H0/ -.302488D0 , 0.195861D-2, -.316302D-5 /,
+ CR11H1/ 0.646422D-3, -.422876D-5, 0.688157D-8 /,
+ CR11H2/ -.332805D-6, 0.223160D-8, -.367713D-11/,
+ CR222 / 0.784980D-2, -.398950D-4, 0.611870D-7 /,
+ CR223 / 0.552066D-2, -.168609D-4, 0.157169D-7 /,
+ CR233 / 0.358783D-2, 0.806674D-5, -.325798D-7 /,
+ CR333 / 0.205130D-2, 0.348880D-4, -.837030D-7 /,
+ CR555 / 0.104711D-2, -.364887D-5, .467095D-8 /,
+ CR117 / 0.736748D-2, -.276578D-4, .343051D-7 /
DATA Z12 / 0.72D0 /, Z13 / -.865D0/,
+ Y12 / 0.92D0 /, Y13 / 0.92D0/, Y123 /1.10D0/,
+ Y115/ 1.2D0/
DATA GM1R0/-2.709328D0/, GM1R1/.021062199D0/,
+ GM2 / 28.0135D0/, GM3 / 44.010D0/,
+ GM5 / 2.0159D0/, GM7 / 28.010D0/,
+ FA /22.414097D0/, FB / 22.710811D0/,
+ RL / 1.292923D0/, T0 / 273.15D0/,
+ H5 / 285.83D0/, H7 / 282.98D0/
+ R /0.0831451D0/
END
C
C

```

Annex G (informative)

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ICS 75.060

Descriptors: natural gas, compressed gas, compression, compression factor, rules of calculation.

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